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Minimum Variance Modelling and Control: Tools and Procedures

by

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A THESIS

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research, for acceptance, a thesis entitled Minimum Variance Modelling and Control: Tools and Procedures submitted by Michael Harold Mac Gregor in partial fulfilment of the requirements for the degree of Master of Science in Process Control.

A master archer hits
A target at a hundred yards because
He skill possesses but, to make to meet
Two arrows in mid-air, head-on, goes far
Beyond the skill of ordinary man.

Dogen Zenji

Abstract

A collection of FORTRAN routines has been developed for use in minimum variance modelling and control. The routines can be grouped into five categories : time series modelling, SISO transfer function plus noise modelling, MIMO transfer function plus noise modelling, unconstrained minimum variance controller design and constrained minimum variance controller design.

Within a category, routines can be grouped by the step at which they are used. For example, transfer function plus noise models require five steps : differencing, prewhitening, model order identification, preliminary estimation and least squares estimation. The main line routine used to perform each step calls on a number of subroutines. After each step has been completed, the analyst must interpret the graphical and numeric outputs produced. The decision then is whether to continue to the next step, or change some input and rerun the current step. That is, the modelling process is interactive and iterative in nature.

Fourteen main line routines are required to run the individual steps in the five categories of tasks which can be performed. These main line routines rely on seventy-eight subroutines to perform the work. Altogether, this amounts to about ten thousand lines of code.

The only way to reliably generate this amount of code is to have some standard practices, and a rich test

environment. The test environment was provided by a "neatness" program called *FTNTIDY, along with a very good checking compiler and run-time system, *IF. Some of the standard practices were:

1. one function per subroutine
2. top-down coding
3. chunk implementation and checkout
4. consistent subroutine call argument format
5. explicit declaration of all variables
6. levels of nesting indicated by indentation
7. errors handled within the routine where they occur

As currently implemented, this set of subroutines is dependent on two features of MTS - the IMSL library, and the plotting library.

Of course, there are other time series packages. The package developed by the author differs from the MTS resident "Time Series Processor" by its extensive use of graphics to represent results. It also has the capability for transfer function plus noise modelling, and can derive minimum variance controllers from transfer function plus noise models. These additions make the package much more useful in control applications.

The purpose of this thesis is to develop the background necessary for the use of this subroutine library. This will serve as an introduction to simple stochastic modelling, and minimum variance control, as well as the foundations of adaptive control.

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Nomenclature

a	random input, disturbance
b	integer number of intervals of delay
c	estimate of autocovariance or cross-covariance
d	degree of differencing
e	prewhitened noise
E	expectation operator
f	number of intervals of pure process delay
I	spectral intensity
n	correlated noise
N	number of observations
$N(0,\sigma^2)$	Gaussian normal process with zero mean and variance σ^2
p	order of autoregressive polynomial $\phi(z^{-1})$
q	order of moving average polynomial $\theta(z^{-1})$
r	order of transfer function denominator, $\delta(z^{-1})$
s	order of transfer function numerator, $\omega(z^{-1})$
u	control input
v	impulse response
V	step response
y	observed output
z^{-1}	unit delay operator
α	prewhitened input
β	prewhitened output
$\gamma(u,u,k)$	autocovariance of series u at lag k
$\gamma(u,y,k)$	cross-covariance from u to y at lag k
$\delta(z^{-1})$	transfer function denominator

$\theta(z^{-1})$	noise model numerator
$\Pi(z^{-1})$	autoregressive operator
$\rho(u,u,k)$	autocorrelation of series u at lag k
$\rho(u,y,k)$	cross-correlation from u to y at lag k
$\sigma^2(a)$	variance of series a
τ	number of intervals of lag
$\phi(z^{-1})$	noise model denominator
$\phi(i,i,k)$	partial correlation of order k
χ^2	chi-squared statistic
$\psi(z^{-1})$	moving average operator
$\omega(z^{-1})$	transfer function numerator

1. INTRODUCTION

In practice, estimating the possible return on a computer control application is difficult. Applications are selected on the basis of possible benefits from a change in the mean value of some key variable(s). The aim is to reduce the amount of off-specification product, increase throughput, decrease energy consumption, etc.

But substantial gains can also result from just reducing the variance of a key variable. This can occur when profit is related to the key variable by a nonlinear function.

For example, the ratio of hydrogen to nitrogen (H/N ratio) at the synthesis converter inlet is a key variable in ammonia plants. Figure 1.1 presents a typical plant performance function, as tons per day of production versus H/N ratio, for a given set of operating conditions. This function can be approximated as:

$$y = 997.5 - 937.5(u-2.9)^2 \qquad (1.1)$$

where:

y = tons/day production
u = H/N ratio

Assume that, without computer control, the H/N ratio is 2.9±0.3. Also assume that a combination of gas chromatograph and hydrogen analyzer could be used in a computer control scheme to produce a ratio of 2.9±0.05.

If the distribution of H/N ratio is uniform (all values equally likely), then computer control can change the average production from 960.0 tons/day, to 996.5 tons/day.

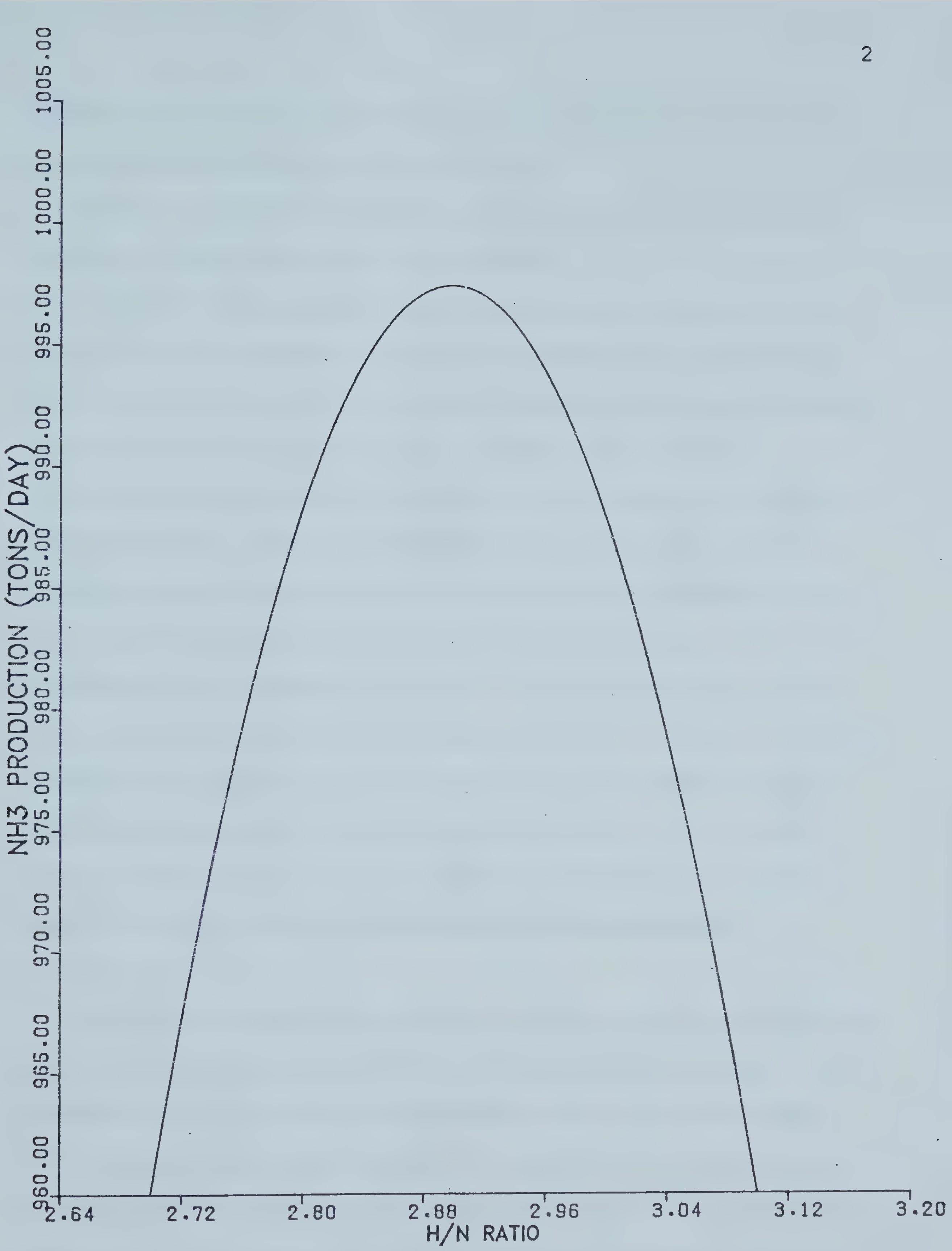

Figure 1.1 Ammonia Plant Performance Function

If the distribution is normal (i.e. Gaussian), the change is from 992.8 tons/day to 996.9 tons/day.

That is, without changing the mean value of the key variable, production can be increased.

In other situations (e.g. fractionator control), the reduced variance permits operation closer to a constraint. Here, the prime benefit is from a change in the mean value, once the variation is reduced to permit the change.

The objective of this thesis is to present, in a clear, concise manner, a set of procedures for achieving minimum variation. The intention is to be reasonably mathematically rigorous. However, there are some basic concepts left undefined (e.g. expected value vs. wide sense expectation). Also, as this thesis is intended to present only one method, concepts not central to the development have been skipped, or merely hinted at (e.g. state estimators). It is hoped that the result is a clearly defined introduction to the broad field of system identification and parameter estimation.

As part of this introduction to the field, an extensive set of tools will be presented. These tools have been implemented as a library of FORTRAN subroutines They deal with progressively more complex situations in modelling. A facility for deriving various types of controller from these models has also been included. The chief advantage of this set of tools is the rich graphical output which is indispensable in this application. Consistency of

implementation and documentation are also important factors recommending the library's use.

However, as well as these tools for offline analysis, tools for online, open-loop experimentation are required. These are not included in the library, since their implementation is highly situation dependent.

In the following chapters, the background necessary for the use of the library will be built up stepwise. Chapter 2 sets out the general notions of model building, and examines various techniques briefly. The correlation method for building input-output models of stochastic plants is then outlined. The foundation of the correlation method is examined more closely in Chapter 3. This chapter sets out three fundamental tools - autocorrelation, partial autocorrelation, and power spectrum. This is the basic toolkit for both time series and transfer function modelling. (Time series modelling is not central to this thesis, but the technique is of great significance. The topic is detailed in Appendix A.) Transfer function plus noise modelling (Chapter 4) follows naturally from Chapter 3. Here, definition of the modelling procedure is completed, and illustrated with an example.

Finally, Chapter 5 addresses the problem of deriving a control law from the plant model. The chapter ends with an illustration of control of the plant modelled in Chapter 4. Chapter 6 presents a series of conclusions and observations on the method.

2. MODELLING STOCHASTIC PLANTS

In this chapter, we will introduce some basic concepts and terminology. First, we present a few categories into which models may be set. Our purpose is to indicate the nature of the models and techniques to be developed. Next, two important methods for describing systems - via state space and transfer function models - are considered briefly. These first sections serve to indicate the general characteristics of the models to be used, and to specify their form. The remaining sections outline procedures which can be used in the building of these models.

2.1 Categories of Models

There are two basic approaches to modelling the dynamic behavior of a system. The first approach could be called theoretical model building. It requires the following steps:

1. Apply basic conservation laws to the process being studied.
2. Derive the ordinary or partial differential/difference equations describing those aspects of the system's behavior which are of interest.
3. Estimate any unknown model parameters.
4. Verify and test the model.

The second approach is experimental determination of the system model, on the basis of input-output data. In this case we obtain a representation only of the observable and controllable part of the system.

For an existing plant, the best "model" is the plant itself. That is, experimental methods will involve the whole plant (valve positioners, piping, distributor plates, etc.) Theoretical models can never be fully descriptive, but are indispensable for predicting either the behavior of new plants, or the results of extreme changes in operating conditions.

This work will concentrate on experimental models. Further, the models considered will be written in discrete time, rather than continuous time, to allow for:

1. slow measurements (e.g. laboratory analyses)
2. time-shared instruments (e.g. gas chromatographs)
3. use of digital computers in data acquisition and control

Models can also be differentiated on the basis of whether or not they attempt to deal with "noise". In the deterministic case, either there is no noise, or it is negligible. Strejc (1981) presents a summary of the most common deterministic methods. With such methods, evaluation of plant measurements yields exact values for model parameters.

Techniques for developing deterministic models fail at low signal to noise ratios. In this region, system response to a test input cannot easily be distinguished from the system response to the noise that is normally present.

Stochastic models are based on statistical methods, to account for the effects of noise. This noise may be assumed to act at various places in the system (input, measurement, etc.) The noise itself is usually unmeasureable. Evaluations

of plant measurements yield only estimates of the parameters in the plant model. To apply such methods, we should have some notion as to what characterizes a "good" estimator. Some definitions of desirable properties follow:

1. Unbiasedness: Let $\hat{\theta}$ be an estimate of a parameter vector θ. If $E\{\hat{\theta}\} = \theta$, then θ is an unbiased estimate of θ. (E denotes expected value.)
2. Consistency: The estimate $\hat{\theta}$ converges in probability to θ as the number of samples, N, increases.

   $$\lim_{N\to\infty} \{\Pr(|\hat{\theta} - \theta|) = 0\} = 1$$

   Consistency implies unbiasedness, but not vice versa.
3. Efficiency: $\hat{\theta}$ is an efficient estimate if no other unbiased estimator has smaller variance than $E\{(\hat{\theta}-\theta)^T(\hat{\theta}-\theta)\}$.
4. Sufficiency: A sufficient estimator contains all the information in the observations regarding the parameters to be estimated. A sufficient estimate $\hat{\theta}$ of θ, based on the sample vector Y, is such that the conditional expectation $E\{\hat{\theta}|Y\}$ is independent of θ.

Estimators have been characterized by Strejc (1981) according to the error cost function and probabilistic concept as follows:

1. Bayes estimation (Ho and Lee,(1964); Peterka(1978))
2. Maximum likelihood (Deutsch,(1965); Astrom,(1980))
3. Markov estimate (Deutsch,(1965))
4. Stochastic approximation (Kiefer and Wolfowitz,(1952))
5. Least squares (Strejc,(1980))

6. Weighted least squares (Deutsch,(1965))
7. Generalized least squares (Eykhoff,(1974); Hastings-James and Sage,(1969))
8. Extended least squares (Young and Hastings-James,(1970))
9. Square root filtering (Peterka,(1975))
10. Kalman-Bucy filtering (Kalman and Bucy,(1967))
11. Instrumental variables (Kendall and Stuart,(1961); Young and Jakeman,(1979))

That is, many estimators are available, all with varying strengths. Each has its proper applications. For example, least squares cannot be used in closed loop. Instrumental variables prove their worth in such an application.

Finally, models can be characterized as parametric or nonparametric. The essential difference is that parametric models can be economic in their use of parameters. They assume some knowledge of the plant's structure. Nonparametric models are prodigal in their use of parameters. When using parametric methods, if the structure of the plant is unknown, an iterative search must be followed. This can sometimes be avoided by the use of a nonparametric method. For example, the step response of a system is a nonparametric model which can yield insight into the system structure.

Such a two step approach to modelling illustrates that we really have two problems to consider. First is the problem of identification of the plant structure. The second problem is the estimation of the unknown parameters. Two

families of models commonly used are state space and transfer function, or input-output, models.

2.2 State Space Models

The behavior of a linear dynamic stochastic system can be described by the state variable model :

$$\begin{aligned} x(k+1) &= \phi(k+1,k)x(k) + \Psi(k+1,k)u(k) + \Gamma(k+1,k)w(k) \\ y(k+1) &= H(k+1)x(k+1) \\ z(k+1) &= y(k+1) + v(k+1) \end{aligned} \qquad (2.1)$$

In this model, x is the state vector, which is sufficient to specify the position of the system. u is the forcing or control vector; w is the disturbance to the state. y is the true system output, while z is the measurement corrupted by noise v.

The state vector, control vector and measurement are all zero mean with dimensions s, t, and r. The sequences $\{v(k)\}$ and $\{w(k)\}$ are independently distributed with zero mean, and covariances V and W respectively.

This type of model can be derived from a theoretical analysis of the process. The state variables may or may not represent observable and/or controllable system attributes. It can be shown (Kalman,(1963)) that there are an infinite number of state representations of the same system. This is due to the fact that the relationship between the input u, and the output y is not affected by a nonsingular linear transformation of state variables. Two models in the form of Equations (2.1) are said to be equivalent if:

1. Their input-output relationships are the same for the

case of no noise. $(v = w = 0)$

2. The statistical properties of the outputs of the unforced systems are the same. $(u = 0)$

2.3 Input-Output Models

Besides simply changing the state vector, there is another transformation of Equations (2.1) which is of interest. By applying the Kalman filter theorem to Equations (2.1), we obtain:

$$\begin{aligned} \hat{x}(k+1) &= \Phi(k+1,k)\hat{x}(k) + \Psi(k+1,k)u(k) + K(k+1)a(k) \\ y(k) &= C(k)\hat{x}(k) + D(k)u(k) + a(k) \end{aligned} \tag{2.2}$$

where $\hat{x}(k)$ is the conditional expectation of $x(k)$, given $y(k-1)$, $y(k-2)$, ... and $a(k)$ is independently randomly distributed with zero mean, and covariance R. Equation (2.2) reduces to:

$$y(k) = \frac{B(z^{-1})}{A(z^{-1})} u(k) + \frac{C(z^{-1})}{A(z^{-1})} a(k) \tag{2.3}$$

for systems with one input and one output (Eykhoff,(1974)), As before, y and u are zero mean; a is independently randomly distributed.

The common denominator in Equation (2.3) implies that both the input, u, and the noise, a, are processed along different paths of the same system. Generalizing slightly to avoid this assumption, we obtain:

$$y(k) = \frac{\omega(z^{-1})}{\delta(z^{-1})} z^{-b} u(k) + \frac{\theta(z^{-1})}{\phi(z^{-1})} a(k) \tag{2.4}$$

where the polynomials are defined as:

$$\begin{aligned} \omega(z^{-1}) &= \omega(0) - \Sigma\omega(i)z^{-i} & i &= 1, \ldots, s \\ \delta(z^{-1}) &= 1 - \Sigma\delta(i)z^{-i} & i &= 1, \ldots, r \\ \theta(z^{-1}) &= 1 - \Sigma\theta(i)z^{-i} & i &= 1, \ldots, q \end{aligned} \tag{2.5}$$

$$\phi(z^{-1}) = 1 - \Sigma\phi(i)z^{-i} \qquad i = 1, \ldots, p$$

and b is the number of whole periods of delay.

Equation (2.4) can also be obtained by representing the deterministic dynamic behavior of the system as the linear filter:

$$y(k) = \Sigma v(i)u(k-i) \qquad i = 0, \ldots, \infty \qquad (2.6)$$

in which the output, y, is represented as a linear combination of a series of impulse response weights, {v(i)}, scaled by the input {u(k-i)}. This is analogous to the convolution integral for continuous systems. Making use of operator notation, Equation (2.6) becomes:

$$y(k) = v(z^{-1})u(k), \; v(z^{-1}) = \Sigma v(i)z^{-i} \qquad i = 0, \ldots, \infty \qquad (2.7)$$

The operator $v(z^{-1})$ is called the transfer function of the filter. To parameterize the system somewhat more economically, $v(z^{-1})$ can be represented as the rational operator:

$$v(z^{-1}) = \frac{\omega(z^{-1})}{\delta(z^{-1})} z^{-b} \qquad (2.8)$$

where the value for b reflects the fact that one or more of the initial v(i) may be zero. Substituting Equation (2.8) back into Equation (2.7):

$$y(k) = \frac{\omega(z^{-1})}{\delta(z^{-1})} z^{-b}u(k) \qquad (2.9)$$

To include the effects of noise on the output signal, let:

$$y(k) = \frac{\omega(z^{-1})}{\delta(z^{-1})} z^{-b}u(k) + n(k) \qquad (2.10)$$

where {n(k)} is an independently, randomly distributed sequence.

The noise sequence may in turn be modelled as the output of a linear filter with random input:

$$n(k) = \frac{\theta(z^{-1})}{\phi(z^{-1})} a(k) \qquad (2.11)$$

Thus, we arrive back at Equation (2.4):

$$y(k) = \frac{\omega(z^{-1})}{\delta(z^{-1})} z^{-b} u(k) + \frac{\theta(z^{-1}) a(k)}{\phi(z^{-1})} \qquad (2.4)$$

2.4 Frequency Response Analysis

Given a restricted class of models to consider (e.g. state space or input-output), the task in a particular application will be to define the system parameters. Historically, this began with frequency response analysis of transfer functions. The simplest case is that of a sine wave forcing to a linear process with noise-free output. Here, the system's amplitude and phase response can be determined from a recording of the input, u, and output, y:

$$|G(j\omega)| = \frac{Y}{U} \qquad \measuredangle G(j\omega) = -\frac{t}{T}\, 360° \qquad (2.12)$$

where T is the period of the input, and t is the amount of time by which the output lags the input. The amplitude ratio and phase angle, ϕ, are related to the transfer function by:

$$G(j\omega) = |G(j\omega)| e^{j\phi} \qquad (2.13)$$

Both depend on the input frequency. The transfer function can, in principle, be found from the response of the process over the entire range of frequencies, $0 \le \omega \le \infty$.

There are two common graphical means of representing frequency response. The first is a pair of plots - amplitude ratio and phase angle versus frequency. This is called the

Bode diagram. The second is a polar plot of $G(j\omega)$ in the complex plane, called the Nyquist diagram.

Frequency response methods have become more practical with the advent of digital spectral analysis, and numerical Fourier transforms. However, these methods will give satisfactory results only if the output signal to noise ratio is very high.

Jenkins and Watts (1968), and Wellstead (1981) describe nonparametric techniques of spectral analysis in detail. Ljung and Glover (1981) contrast the features of frequency and time domain methods. They conclude that the two approaches complement each other.

2.5 Impulse Response Analysis

If we use an input signal of the form:

$$u(t) = k\delta(t) \tag{2.14}$$

where δ is the Dirac delta, the process output will be:

$$y(t) = kv(t) + n(t) \tag{2.15}$$

where $v(t)$ is the impulse response, and $n(t)$ is noise corrupting the output. In practice, $\delta(t)$ has to be approximated by impulse functions with short but finite duration, and limited amplitude. In this case, inversion of the convolution:

$$y(t) = \int_0^\infty v(\tau)u(t-\tau)d\tau \tag{2.16}$$

will determine the impulse response. However, deconvolution may suffer significantly from ill-conditioned inputs and/or

nonnegligible noise (Rake,(1980)). Thus, the approximate approach is impractical.

The currently accepted approach to impulse response analysis involves the use of statistical methods.

2.6 Correlation Methods

Correlation methods are based on the analysis of autocovariance and cross-covariance functions of stochastic processes.

The autocovariance function is an important statistical property of a process, defined as:

$$\gamma(u,u,t_1,t_2) = E[u(t_1)u(t_2)] \qquad (2.17)$$

where the operator "E" denotes expected value. If the stochastic process is weakly stationary, a term that will be defined in detail later, then the covariance depends only on the time difference $|t_1 - t_2|$. Setting this equal to τ,

$$\gamma(u,u,\tau) = E[u(t)u(t+\tau)] \qquad (2.18)$$

Similarly, the cross-covariance between two weakly stationary processes is:

$$\gamma(u,y,\tau) = E[u(t)y(t+\tau)] \qquad (2.19)$$

On the ergodic hypothesis, the time average equals the ensemble average. So, for a weakly stationary, ergodic process u(t),

$$\begin{aligned}\gamma(u,u,\tau) &= E[u(t)u(t+\tau)] \\ &= \{\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} u(t)u(t+\tau)d\tau\} \qquad (2.20)\end{aligned}$$

Similarly, the cross-covariance can be defined as:

$$\gamma(u,y,\tau) = \{\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} u(t)\, u(t+\tau)d\tau\} \qquad (2.21)$$

Using Equation (2.20), the following properties for the autocorrelation function are evident:

1. It is an even function of τ.
2. $\gamma(u,u,0)\geq|\gamma(u,u,\tau) \quad \forall\ \tau$
3. $\gamma(u,u,0) = E[u^2(t)] = \sigma^2(u)$.
4. If a signal has only random components, then $\gamma\to0$ as $\tau\to\infty$.
5. A given autocovariance may give rise to an infinite number of time functions, but any given function of time gives rise to only one autocovariance.

Similarly, the cross-covariance has the following properties:

1. $\gamma(u,y,\tau)\neq\gamma(u,y,-\tau)$
2. $\gamma(u,y,\tau) = \gamma(y,u,-\tau)$
3. γ is not necessarily maximum at $\tau=0$.

The integral definitions in Equations (2.20) and (2.21) become immediately useful if we wish to examine the connection between these functions and the impulse response. Starting with the convolution integral:

$$y(t+T) = \int_{-\infty}^{\infty} v(\tau)u(t+T+\tau)\, d\tau \qquad (2.22)$$

where T is some fixed constant, multiplying by u(t) and taking expectations:

$$\gamma(u,y,T) = \int_{-\infty}^{\infty} v(\tau)\gamma(u,u,\tau+T)d\tau \qquad (2.23)$$

In discrete form:

$$\gamma(u,y,k) = \sum_{i=-\infty}^{\infty} v(i)\gamma(u,u,i+k) \tag{2.24}$$

That is, if we apply an input signal of autocovariance $\gamma(\tau)$, the impulse response can be obtained by deconvolution. In particular, white noise has autocovariance:

$$\gamma(u,u,\tau) = k\delta(\tau) \tag{2.25}$$

Now Equation (2.23) becomes:

$$\gamma(u,y,\tau) = k\int_{-\infty}^{\infty} v(\tau)\delta(\tau+T)d\tau$$

$$\gamma(u,y,\tau) = kv(\tau) \tag{2.26}$$

By adding white noise to the normal operating input signal, we obtain a cross-covariance proportional to the impulse response. In performing such a test, it is our choice whether to apply a continuous or periodic signal. Wellstead (1981) shows that, using a periodic test signal, with impulse-like autocovariance over the period, reduces the variability of the estimated impulse response. This is the motivation for the use of "pseudo-noise" test signals, particularly pseudo-random binary signals (PRBS).

In a manner similar to the above development for impulse response analysis, we can examine the connection between frequency response analysis and correlation methods. In brief, we can estimate a system's frequency response from the autospectrum, $S(u,u,\omega)$, and cross-spectrum, $S(u,y,\omega)$:

$$S(u,u,\omega) = G(j\omega)S(u,u,\omega) \tag{2.27}$$

where $S(u,u,\omega)$ and $S(u,y,\omega)$ are the Fourier transforms of $\gamma(u,u,\tau)$ and $\gamma(u,y,\tau)$ respectively.

Thus, correlation methods can form the basis for both impulse and frequency response analysis. Correlation methods have the advantage of noise immunity. Both impulse and frequency response analysis yield nonparametric models. These are generally useful in exposing system structure. However, parametric models are much more useful in summarizing or predicting behavior.

2.7 Parameter Estimation Methods

To apply a parametric method in system identification, a certain model structure must first be assumed. Then the model parameters are estimated by minimizing an error between model and process responses. For parametric identification methods, an iterative search must be used if the correct model structure is not known in advance. In contrast, nonparametric methods yield the final model directly.

We presented a general input-output description of a linear process earlier:

$$y(k) = \frac{\omega(z^{-1})}{\delta(z^{-1})} z^{-b} u(k) + \frac{\theta(z^{-1})a(k)}{\phi(z^{-1})} \qquad (2.4)$$

The objective of the various methods is to estimate the parameters of the polynomials in Equation (2.4) from input-output data. In Table 2.1, the important properties and computational features of several methods are summarized (Isermann,(1980)). Performance comparisons have been based on simulations (Saridis,(1974)); (Isermann et al,(1974)) and analytical methods (Soderstrom et al,(1978)).

METHOD	PROCESS	NOISE	REMARKS	PROPERTIES
Least Squares (LS)	-	$1/\phi$	Autoregressive	Small computational expense. Available for short identification time if noise acts on the process. Sensitive to unknown mean. Biased estimates for real noise.Reliable convergence for RLS.
	-	θ	Moving average	
	ω/δ	$1/\delta$	Special noise model	
Generalized Least Squares (GLS)	ω/δ	$1/\delta F$		Large computational expense. Biased estimates possible.
Extended Least Squares (ELS)	ω/δ	θ/δ		RELS convergence similar to RML.
Maximum Likelihood (ML)	ω/δ	θ/δ	Special denominator in noise model	Large computational expense. RML slow convergence in starting phase. Good performance for special noise models.
Instrumental Variable (IV)	ω/δ	θ/ϕ	Most general noise model	Medium to small computational expense. Good performance for a wide range of noise models. RIV not reliably convergent - start with RLS recommended.
Correlation and Least Squares (COR-LS)	ω/δ	θ/ϕ	Most general noise model	Small computational expense. Good performance for a wide range of noise models. Search for model order possible.

Table 2.1 Parameter Estimation Methods
Isermann, (1980)

Modelling is generally an iteration through the following steps:

1. Specify the application for the model.
2. Use any a priori knowledge to specify general features of the system. (e.g. linearity, time constants, delays, etc.)
3. Choose an identification method.
4. Select input signals, sampling time, length of experiment.
5. Generate measurements.
6. Identify model structure and estimate parameters.
7. Test the candidate model.
8. Accept the model, or change the experimental or model structure.

In addition to choosing an identification method, many other tasks have to be performed. The general procedure consists of several steps, requiring both an understanding of the process, and a strong theoretical background.

2.8 Summary

The purpose of this chapter was to provide the terminology and motivation for the developments to follow.

First, we examined the various categories of models. These categories provide the referents for all further developments. In this work, we will be concerned with experimental, discrete stochastic models.

Two families of models were next examined. State space models were outlined, since they are a significant landmark in modelling. As demonstrated, they are closely related to input-output models. In the remainder of this work, we will deal only with input-output models.

The difficult step in building input-output models is identifying their structure. We will use nonparametric methods to identify system structure, and then use parameter estimation within this structure. The nonparametric techniques used classically are frequency and impulse response analysis. However, neither analysis, in its original form, deals adequately with noise. Their connection with correlation methods, which deal explicitly with noise, will be taken advantage of in the following chapters.

This establishes the necessary background. Correlation methods will be used to take us through the difficult initial step of model structure identification. Once a tentative model structure has been established, nonlinear least squares estimation for an input-output model will be used.

This method of attack is referred to by Isermann as COR-LS.

3. BUILDING THE NOISE MODEL

In this chapter, we will develop the foundations of the correlation - least squares method. First, we consider briefly the interpretation of the class of models selected. These models are based on two representations - the pure autoregressive and pure moving average forms. There are several interesting parallels between the two forms. One parallel appears during a close look at convergence conditions. Another appears as we consider identification tools for the two forms. The autocorrelation function is related to the moving average form; the partial autocorrelation is related to the autoregressive form. These two functions are defined, and their application is demonstrated in an example. One additional tool - the power spectrum - is also introduced, and applied in the same example.

The class of models which we propose to use:

$$y(k) = \frac{\omega(z^{-1})}{\delta(z^{-1})} z^{-b} u(k) + \frac{\theta(z^{-1}) a(k)}{\phi(z^{-1})} \qquad (3.1)$$

consists of two parts. The first term describes the deterministic part of the plant. The second term describes the effects of stochastic signals which are always present, passing through the plant. The stochastic signals will be referred to as noise.

Identification of the noise model will be considered first. This will require several concepts and tools which will be developed further in modelling the plant transfer function.

The noise model subproblem is of considerable interest in itself, and falls within the general topic of time series analysis. To begin with, we should determine how to interpret the class of models:

$$n(k) = \frac{\theta(z^{-1})}{\phi(z^{-1})} a(k) \tag{3.2}$$

where

$$\theta(z^{-1}) = 1 - \Sigma\theta_i z^{-i} \qquad i = 1, \ldots, q$$
$$\phi(z^{-1}) = 1 - \Sigma\phi_i z^{-i} \qquad i = 1, \ldots, p$$
$$a(k) = N(0,\sigma^2(a))$$

Yule (1927) proposed that a series of observations which appear to follow some pattern can be regarded as having been generated from a series of independent shocks. That is, we can picture the process noise as having been generated from white noise passing through a linear filter.

In Equation (3.2), we wrote the filter as a rational operator to economize on parameters, by using both past inputs and outputs. The pure input formulation:

$$n(k) = \Psi(z^{-1})a(k) \tag{3.3}$$

where

$$\Psi(z^{-1}) = 1 + \Sigma\psi_i z^{-i} \qquad i = 1, \ldots, \infty$$

is referred to as a moving average (MA) process. This is somewhat of a misnomer, in that the weights do not necessarily sum to unity.

The pure output formulation:

$$\Pi(z^{-1})n(k) = a(k) \tag{3.4}$$

where

$$\Pi(z^{-1}) = 1 + \Sigma\pi_i z^{-i} \qquad i = 1, \ldots, \infty$$

is referred to as an autoregressive (AR) process, since the output is being regressed on itself.

3.1 Stationarity and Invertibility

Consider a process written in pure MA form:

$$n(k) = \Sigma\psi_j a(k-j) \quad j = 0, \ldots, \infty \tag{3.5}$$

where both a(k) and n(k) are zero mean. The variance of the process is defined as:

$$\sigma^2(n) = E(n^2(k)) \tag{3.6}$$

Substituting for n(k) from Equation (3.5):

$$\sigma^2(n) = E[\Sigma\psi_j^2\ a^2(k-j)] \quad j = 0, \ldots, \infty \tag{3.7}$$

Also, by definition:

$$E(a^2(k)) = \sigma^2(a) \tag{3.8}$$

Substituting Equation (3.8) into Equation (3.7) and simplifying:

$$\sigma^2(n) = \sigma^2(a)\Sigma\psi_j^2 \quad j = 0, \ldots, \infty \tag{3.9}$$

which makes sense as long as the series sum converges.

So, for n(k) to have finite variance, $\Psi(z^{-1})$ must converge for $|z^{-1}| \leq 1$. This is known as the stationarity condition.

If we consider the pure AR process:

$$\Pi(z^{-1})n(k) = a(k) \tag{3.10}$$

then following a similar procedure as above, we obtain:

$$\sigma^2(a) = \sigma^2(n)\Sigma\pi_j^2 \quad j = 0, \ldots, \infty \tag{3.11}$$

This says that for the observed series n(k) to have arisen from a series of finite variance, then $\Pi(z^{-1})$ must converge for $|z^{-1}| \leq 1$. This is known as the invertibility condition.

But since we have elected to use finite order polynomials, what is the motivation for considering these infinite order polynomials ? Via polynomial division, a

finite order moving average process can be represented as an infinite order autoregressive process. And a finite order AR process can likewise be represented as infinite order MA.

So the stationarity condition that $\Psi(z^{-1})$ converge, where:

$$n(k) = \Psi(z^{-1})a(k) \tag{3.12}$$

is important for AR processes only. (A finite order moving average operator will always converge.)

Conversely, the invertibility condition that $\Pi(z^{-1})$ converge, where:

$$\Pi(z^{-1})n(k) = a(k) \tag{3.13}$$

is important only for MA processes. For example, consider the MA process of order one (MA(1)) :

$$n(k) = (1-\theta z^{-1})a(k) \tag{3.14}$$

where $|\theta|<1$. This can be represented as an infinite order AR process (AR(∞)) :

$$\Pi(z^{-1})n(k) = a(k) \tag{3.15}$$

where $\pi_j = -\theta^j$. The invertibility condition is satisfied, given $|\theta|< 1$.

If we consider representing the MA(q) process:

$$n(k) = (1 - \Sigma\theta_i z^{-i})a(k) \quad i = 1, \ldots, q \tag{3.16}$$

as an autoregressive process:

$$\theta(z^{-1})n(k) = a(k) \tag{3.17}$$

where the original polynomial can be factorized as:

$$\theta(z^{-1}) = \Pi(1 - T_i z^{-1}) \quad i = 1, \ldots, q \tag{3.18}$$

then the inverted polynomial can be represented as:

$$\theta^{-1}(z^{-1}) = \Sigma \frac{A_i}{1 - T_i z^{-1}} \qquad i = 1,\ldots,q \tag{3.19}$$

which converges only for $|T_i|<1$. The roots of $\theta(z^{-1})$ must lie outside the unit circle for invertibility.

If we consider representing the AR(p) process:

$$(1 - \Sigma\phi_i z^{-i})n(k) = a(k) \quad i = 1, \ldots, p \tag{3.20}$$

as a moving average process:

$$n(k) = \phi^{-1}(z^{-1})a(k) \tag{3.21}$$

with the original polynomial factorized as:

$$\phi(z^{-1}) = \Pi(1 - P_i z^{-1}) \tag{3.22}$$

then the inverted polynomial is:

$$\phi^{-1}(z^{-1}) = \Sigma \frac{A_i}{1 - P_i z^{-1}} \quad i = 1,\ldots,p \tag{3.23}$$

which converges for $|P_i|< 1$. The roots of $\phi(z^{-1})$ must lie outside the unit circle for stationarity.

3.2 Further Remarks on Stationarity

It should be stressed that stationarity implies that the process maintains statistical equilibrium.

Strict stationarity implies that the mean, variance and all higher order moments are constant. Stationarity of order k means that all moments up to order k are constant. Since only the first two moments are necessary to define a Gaussian distribution, assuming normality plus stationarity of order 2 implies strict stationarity.

However, considering the typical changes in an industrial plant, it is perhaps unreasonable to assume that process disturbances will have a fixed mean. If we consider:

$$(1 - \phi z^{-1})n(k) = a(k) \tag{3.24}$$

with $|\phi|< 1$, the process is stable. With $|\phi| > 1$, n(k) grows

exponentially. But, if $\phi = 1$, then:

$$(1 - z^{-1})n(k) = a(k) \tag{3.25}$$

or:

$$n(k) - n(k-1) = a(k) \tag{3.26}$$

so that now we are concerned only with successive changes in $n(k)$, rather than absolute values.

That is, we model the changes in $n(k)$. The observed process noise is considered the result of integrating these changes.

If we define:

$$\nabla = (1 - z^{-1}) \tag{3.27}$$

then Box and Jenkins (1976) refer to the model:

$$\nabla^d n(k) = \frac{\theta(z^{-1})}{\phi(z^{-1})} a(k) \tag{3.28}$$

as an autoregressive, integrated moving average model of order (p,d,q). This is abbreviated as ARIMA(p,d,q).

3.3 Autocorrelation

There are three basic tools used in ARIMA model identification. The first of these is the autocorrelation function. It is related to the less general concept of variance. Variance is defined as:

$$\sigma^2(n) = E[n^2(k)] \tag{3.29}$$

where

$n(k) = \tilde{n}(k) - \bar{n}$
$\tilde{n}(k)$ = observed value
$\bar{n}$ = mean value

Variance is estimated as:

$$s^2(n) = (1/N)\Sigma n_i^2 \quad i = 1, \ldots, N \tag{3.30}$$

The more general autocovariance is defined as:

$$\gamma(j) = E[n(k)n(k+j)] \tag{3.31}$$

It is best estimated as:

$$c(j) = (1/N)\Sigma n(i)n(i+j) \quad i = 1, \ldots, N-j \tag{3.32}$$

Note that $\gamma(0) = \sigma^2$.

To obtain the autocorrelation function, we normalize the autocovariance:

$$\rho(j) = \gamma(j)/\gamma(0) \tag{3.33}$$

The autocorrelation of a process is thus independent of its variance.

The autocorrelation function is estimated as:

$$r(j) = c(j)/c(0) \tag{3.34}$$

What does the autocorrelation indicate ? Consider the MA(q) process:

$$n(k) = \theta(z^{-1})a(k) \tag{3.35}$$

Substituting Equation (3.25) into Equation (3.31) we obtain:

$$\begin{aligned}\gamma(j) = E[&(a(k)-\theta(1)a(k-1)-\ldots-\theta(q)a(t-q)) \text{ X} \\ &(a(k-j)-\theta(1)a(k-j-1)-\ldots-\theta a(k-j-q)]\end{aligned} \tag{3.36}$$

For k = 0, we obtain:

$$\gamma(0) = (1+\theta^2(1)+\ldots+\theta^2(q))\ \sigma^2(a) \tag{3.37}$$

and for $k \neq 0$:

$$\gamma(j) = \begin{cases} (-\theta(j)+\theta(1)\theta(j+1)+\ldots+\ \theta(q-j)\theta(q))\sigma^2(a) & , j=1,\ldots q \\ 0 & , j>q \end{cases} \tag{3.38}$$

We have used the fact that:

$$E[a(k)a(k-i)] = \begin{cases} \sigma^2(a) & , i = 0 \\ 0 & , i \neq 0 \end{cases} \tag{3.39}$$

to obtain these results. If we look at the autocorrelation function:

$$\rho(j) = 0 \qquad , j > q \tag{3.40}$$

That is, for a pure moving average process, the theoretical autocorrelation function is zero beyond lag q. Since a finite order autoregressive process is equivalent to an MA(∞) process, its theoretical autocorrelation function will be infinite in extent.

In practice, we will estimate $\rho(k)$ from a series of measurements. We will need some criterion for deciding whether $\rho(k)$ is effectively zero beyond a given lag. The variance of the estimate $r(k)$ for a stationary normal process, is given by Bartlett (1955) as:

$$\sigma^2(r(j)) \cong (1/N)\Sigma\{\rho^2(i) + \rho(i+j)\rho(i-j) - 4\rho(j)\rho(i)\rho(i-j) + 2\rho^2(i)\rho^2(j)\} \tag{3.41}$$

If the autocorrelation is zero for $k > q$:

$$\sigma^2(r(j)) \cong (1/N)\{1 + 2\Sigma\rho^2(i)\}, \quad i=1, \ldots, q\ , \quad j >> q \tag{3.42}$$

Substituting $r(i)$ for $\rho(i)$, we obtain the large lag standard error of the autocorrelation estimates.

3.4 Partial Autocorrelation

Since the autocorrelation reveals the moving average nature of a process, we might expect another tool to reveal the autoregressive nature of a process. This tool is the partial autocorrelation.

Consider the AR(p) process:

$$\phi(z^{-1})n(k) = a(k) \tag{3.43}$$

where:

$$\phi(z^{-1}) = 1 - \Sigma\phi_i z^{-i} \quad i = 1, \ldots, p \tag{3.44}$$

Changing the notation somewhat, let $\phi(p,j)$ be the j'th

coefficient of an AR(p) process. We now have:

$$\phi(z^{-1}) = 1 - \Sigma\phi(p,i)z^{-i} \quad i = 1, \ldots, p \tag{3.45}$$

If we define the set of autoregression coefficients, $\{\phi(i,i)\}$, as the partial autocorrelation,

$$\phi(i,i) = 0 \ , \ i > p \tag{3.46}$$

for a pure AR(p) process. That is, for a pure autoregressive process, the partial autocorrelation cuts off for $i > p$. Since MA(q) is equivalent to AR(∞), the theoretical partial autocorrelation for a pure moving average process is infinite in extent.

There are two alternatives for estimating the partial autocorrelations. The first is based on a solution in terms of the autocorrelations, called the Yule-Walker equations. Consider the AR(i) process:

$$n(k) = \phi(i,1)n(k-1)+\ldots+\phi(i,i)n(k-i) \ + a(k) \tag{3.47}$$

Multiplying by $n(t-k)$ and taking expectations:

$$\gamma(j) = \phi(i,1)\gamma(j-1)+\ldots+ \phi(i,i)\gamma(j-i) \ , \ j > 0 \tag{3.48}$$

or:

$$\rho(j) = \phi(i,1)\rho(j-1)+\ldots+ \phi(i,i)\rho(j-i) \ , \ j > 0 \tag{3.49}$$

So that:

$$P(k)\Phi(k) = \rho(k) \tag{3.50}$$

where

$$P(k) = \begin{bmatrix} 1 & \rho(1) & \ldots & \rho(k-1) \\ \rho(1) & 1 & \ldots & \rho(k-2) \\ \cdot & \cdot & \cdots & \cdot \\ \rho(k-1) & \rho(k-2) & \ldots & 1 \end{bmatrix}$$

$$\Phi(k)^T = [\phi(k,1) \ \phi(k,2) \ \ldots \ \phi(k,k)]$$
$$\rho(k)^T = [\rho(1) \ \rho(2) \ \ldots \ \rho(k)]$$

These equations are solved for increasing values of k.

Durbin (1960) presents a recursive algorithm for solving Equations (3.50).

However, the Yule-Walker equations are not well conditioned. A more stable alternative is to fit autoregressive models of increasing order to the data, via least squares.

Again, to determine whether a particular value is significant, we need a test. Quenouille (1949) has shown that, assuming the process is AR(p), the estimated partial autocorrelations are approximately independently distributed for i > p. Then:

$$\sigma^2(\phi(i,i)) \cong (1/N),\ i > p \qquad (3.51)$$

where N is the number of observations.

3.5 Power Spectrum

Neither the autocorrelation nor the partial autocorrelation will reveal the presence of periodic components in the observations. The Fourier transform of the autocorrelation yields the power spectrum, which will show periodicities. In particular, a large peak in the low frequency range may indicate a slowly changing level or slope which may be removed by differencing.

Given an odd number of obeservations, N = 2q+1, we fit the Fourier series model:

$$n(k) = \alpha(0) + \Sigma(\alpha(i)c(i,k) + \beta(i)s(i,k) + e(k),\ i=1, \ldots q \qquad (3.52)$$

where:

$$c(i,k) = \cos(2\pi f(i)k)$$
$$s(i,k) = \sin(2\pi f(i)k) \quad f(i) = (i/N)$$

The least squares estimates for α and β are:

$$\begin{aligned} a(0) &= n \\ a(i) &= (2/N)\Sigma n(k)c(i,k) \quad i=1, \ldots, q \\ b(i) &= (2/N)\Sigma n(k)s(i,k) \quad k=1, \ldots, N \end{aligned} \qquad (3.53)$$

Now that the data has been transformed into the frequency domain, we must represent it somehow. The usual technique is to plot signal strength versus frequency. This is known as the signal spectrum. The signal strength, or intensity, at frequency f(i) is defined as:

$$I(f(i)) = (N/2)(a^2(i) + b^2(i)) \quad i=1, \ldots, q \qquad (3.54)$$

For an even number of samples, N, the procedure is modified slightly. Let N = 2q, and:

$$\begin{aligned} a(q) &= (1/N)\Sigma(-1)^k n(k) \quad k=1, \ldots, N \\ b(q) &= 0 \\ I(f(q)) &= Na^2(q) \end{aligned} \qquad (3.55)$$

with a(i), b(i) and I(f(i)) for i = 1, ..., q-1 as before.

For a truly random series:

$$n(k) = \alpha(0) + e(k) \qquad (3.56)$$

That is, the signal will have only a DC component equal to the signal average, plus some error component causing it to vary about this value. In this case, the expected value of I(f(i)) is $2\sigma^2(n)$, distributed as $\sigma^2(n)\chi^2(2)$. (The intensity of white noise is uniform at all frequencies, and equals $2\sigma^2(n)$.)

If there are periodic components in the series, the power spectrum will show an increase of intensity in the vicinity of the frequencies of these components. (See Figure 3.1)

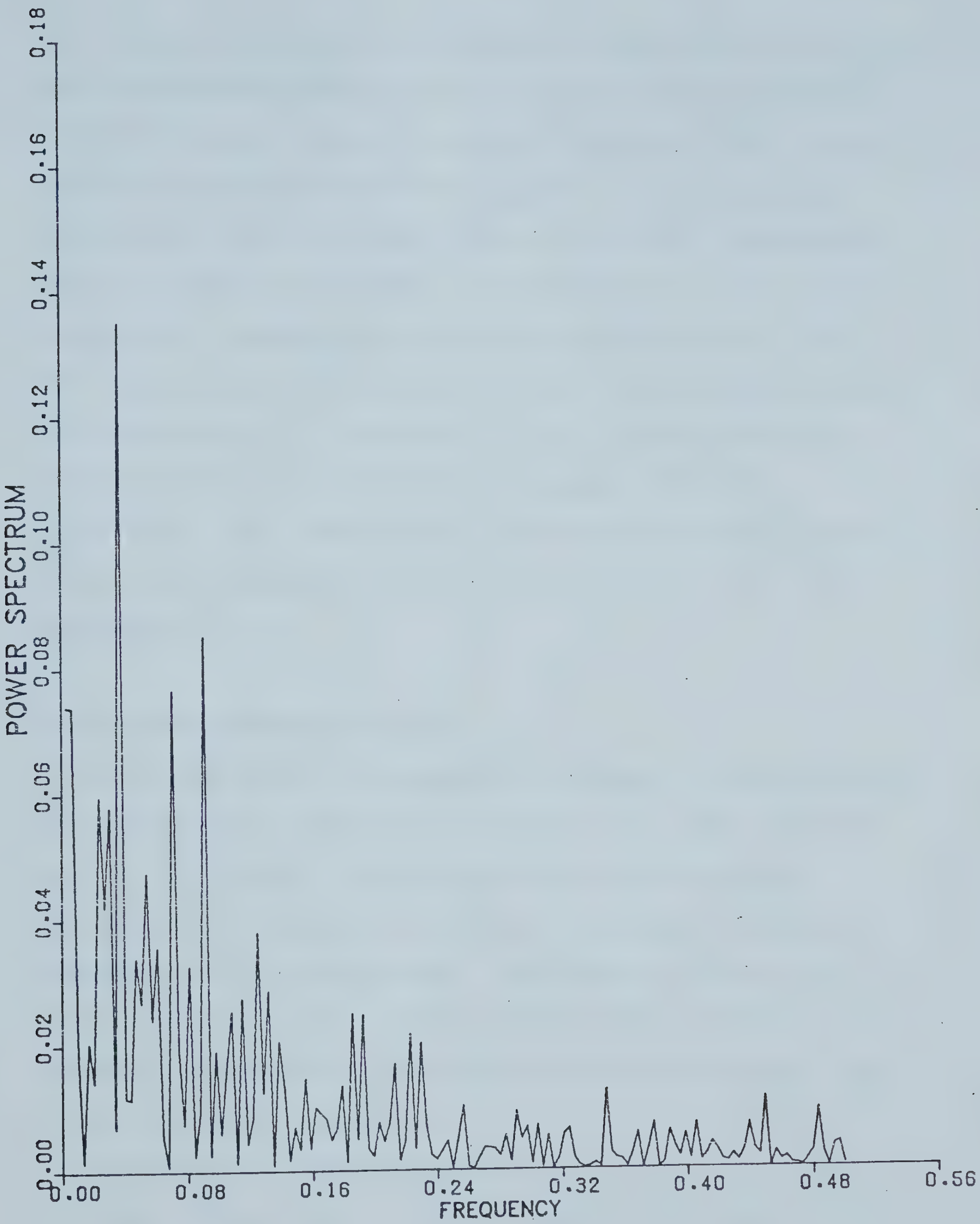

Figure 3.1 Example Power Spectrum

If we integrate and normalize the spectrum, deviations from the expected behavior of white noise can be assessed via the Kolmogorov-Smirnov bounds. (See Figure 3.2) White noise has a uniform frequency content, so its integrated spectrum will be a straight line of slope $2\sigma^2$. Normalizing by σ^2, we obtain a straight line of slope 2. Limit lines can be drawn at distances $\pm K(\epsilon)/\sqrt{q}$ above and below this line. For white noise, an excursion over the limit line will occur with probability ϵ. On Figure 3.2, the lines nearest the central white noise line will be crossed with 10% probability. The lines further out would be crossed by white noise with 1% probability. Approximately, $K(0.01) = 1.63$, and $K(0.1) = 1.22$.

3.6 An Autoregressive Process

In this section, we present an example of identifying a pure AR process. The advantage we have here over the real case is that we will actually specify the underlying process. We will generate a series of samples (termed a "realization" of the process), and then see how well our tools reveal it to us. We will examine both numerical and graphical representations, although we would normally rely on the graphical information.

Consider the AR(2) process:

$$(1-1.16z^{-1}+0.33z^{-2})n(k) = a(k) \quad , \; a(k) = N(0,0.05) \quad (3.57)$$

which has the roots at $z^{-1} = 1.5$ and $z^{-1} = 2$. If we generate a realization of this process using the initial values:

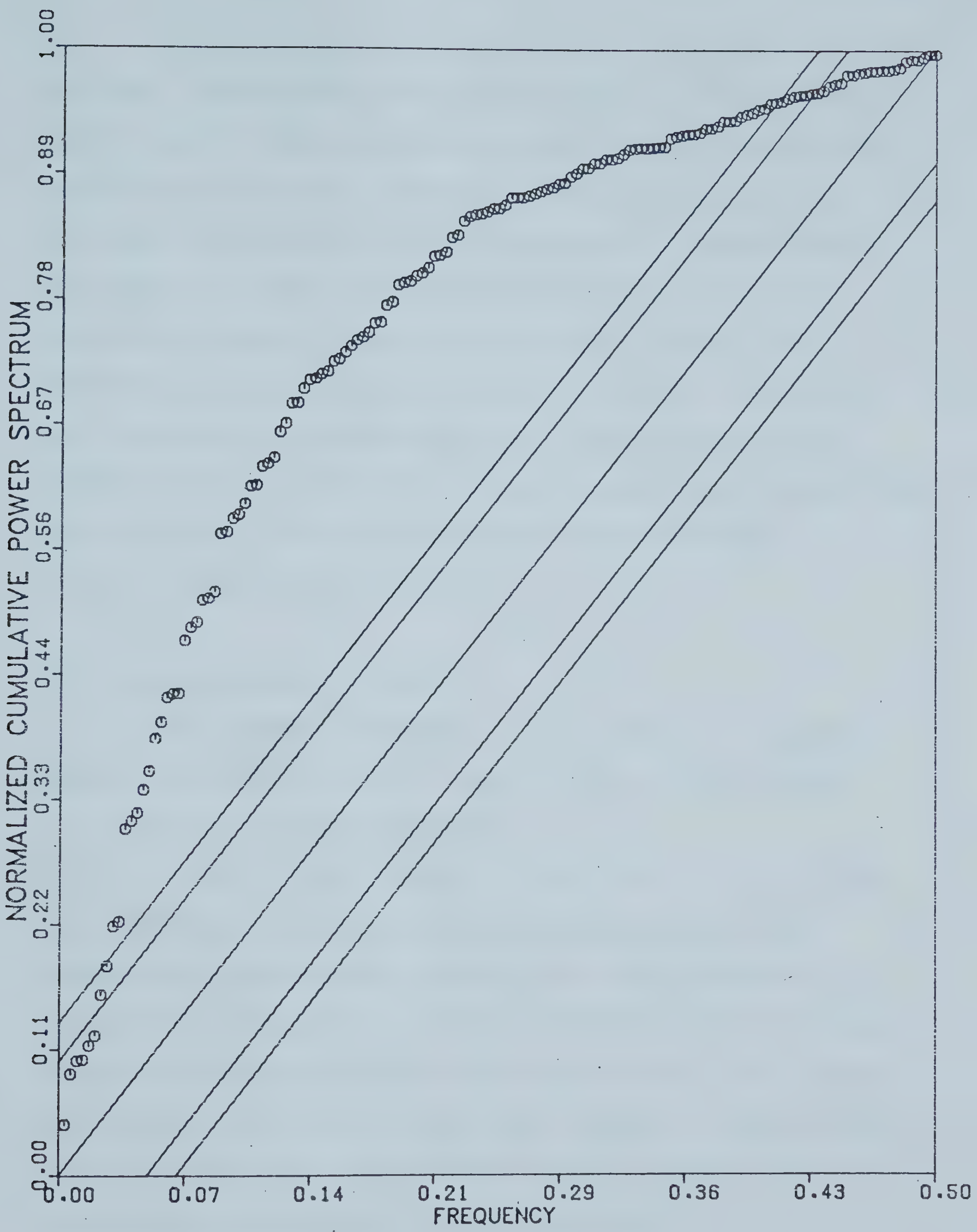

Figure 3.2 Example Normalized Cumulative Spectrum

$$n(-1) = -2.2 \ , \ n(0) = 1.2 \qquad (3.58)$$

we obtain the results presented in Table 3.1. The autocorrelation and partial autocorrelation estimates, with confidence limits, are presented in Figures 3.3 and 3.4. Note that the estimated values in Table 3.1 compare quite well with the theoretical values for this process. The significant results, however, are in the figures. The estimated autocorrelation is significant over a number of lags. This is as it should be for a pure autoregressive process. On the other hand, the partial autocorrelation cuts off after lag 2. This process would be tentatively, correctly, identified as AR(2).

3.7 A Moving Average Process

As for the AR(2) example, we will specify a process, generate a realization, and see how well our tools work.

Consider the MA(2) process:

$$n(k) = (1+1.05z^{-1}+0.8z^{-2})a(k) \quad , \ a(k) = N(0,1) \qquad (3.59)$$

The numerical results are presented in Table 3.2. The estimated autocorrelation and partial autocorrelation are presented in Figures 3.5 and 3.6. As before, the estimates compare favourably with the theoretical values. The partial autocorrelation is significant over a number of lags, while the autocorrelation cuts off after lag 2. Again, this process would be properly identified as MA(2).

3.8 A Mixed Process

Mixed processes are the norm in real applications, and represent the most difficult identification problems. Here, it is not simply a case of one function being continuous, and the other cutting off cleanly. Both judgement and experience are required. An additional complexity is introduced by the possibility of nonstationarity.

	Actual	Estimate		Actual	Estimate
$\rho(1)$	0.872	0.818	$\phi(1,1)$	0.872	0.818
$\rho(2)$	0.682	0.606	$\phi(2,2)$	-0.33	-0.19
$\rho(3)$	0.503	0.429	$\phi(3,3)$	0.0	-0.018

Table 3.1 Results for AR(2)

	Actual	Estimate
$\rho(1)$	0.689	0.643
$\rho(2)$	0.292	0.231
$\rho(3)$	0.0	-0.039

Table 3.2 Results for MA(2)

To test our tools, we use a realization of the ARIMA(1,1,1) process:

$$(1+0.2z^{-1})\nabla n(k) = (1-0.5z^{-1})a(k) \quad , \; a(k) = N(0,1) \qquad (3.60)$$

This can be rearranged as:

$$n(k) = 0.8n(k-1)+0.2n(k-2)+a(k)-0.5a(k-1) \qquad (3.61)$$

The autocorrelation plot (Figure 3.7) is significant over a large number of lags. That this could be due to nonstationarity is confirmed by the large peak near DC in the power spectrum (Figure 3.8).

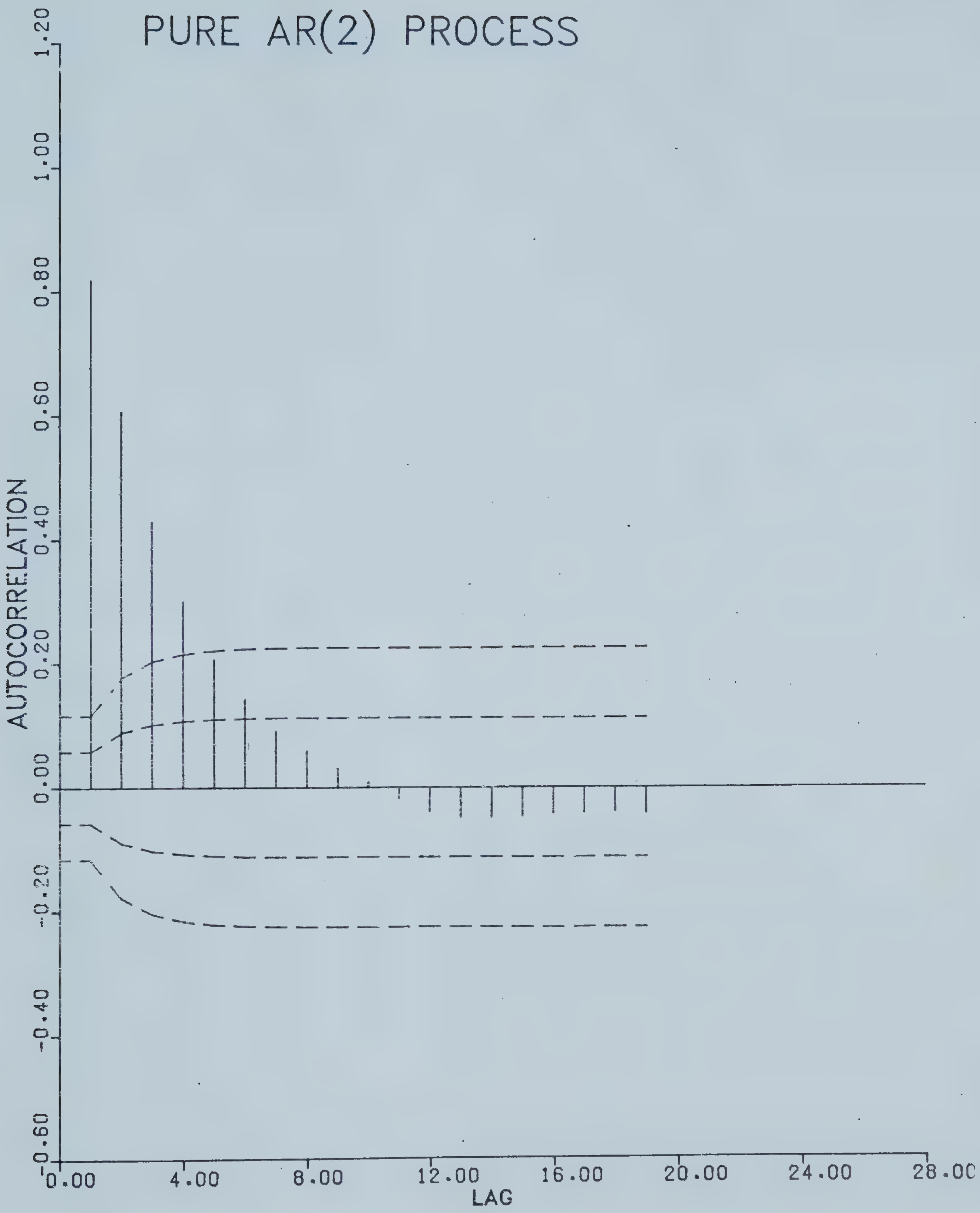

Figure 3.3 AR(2) Autocorrelation

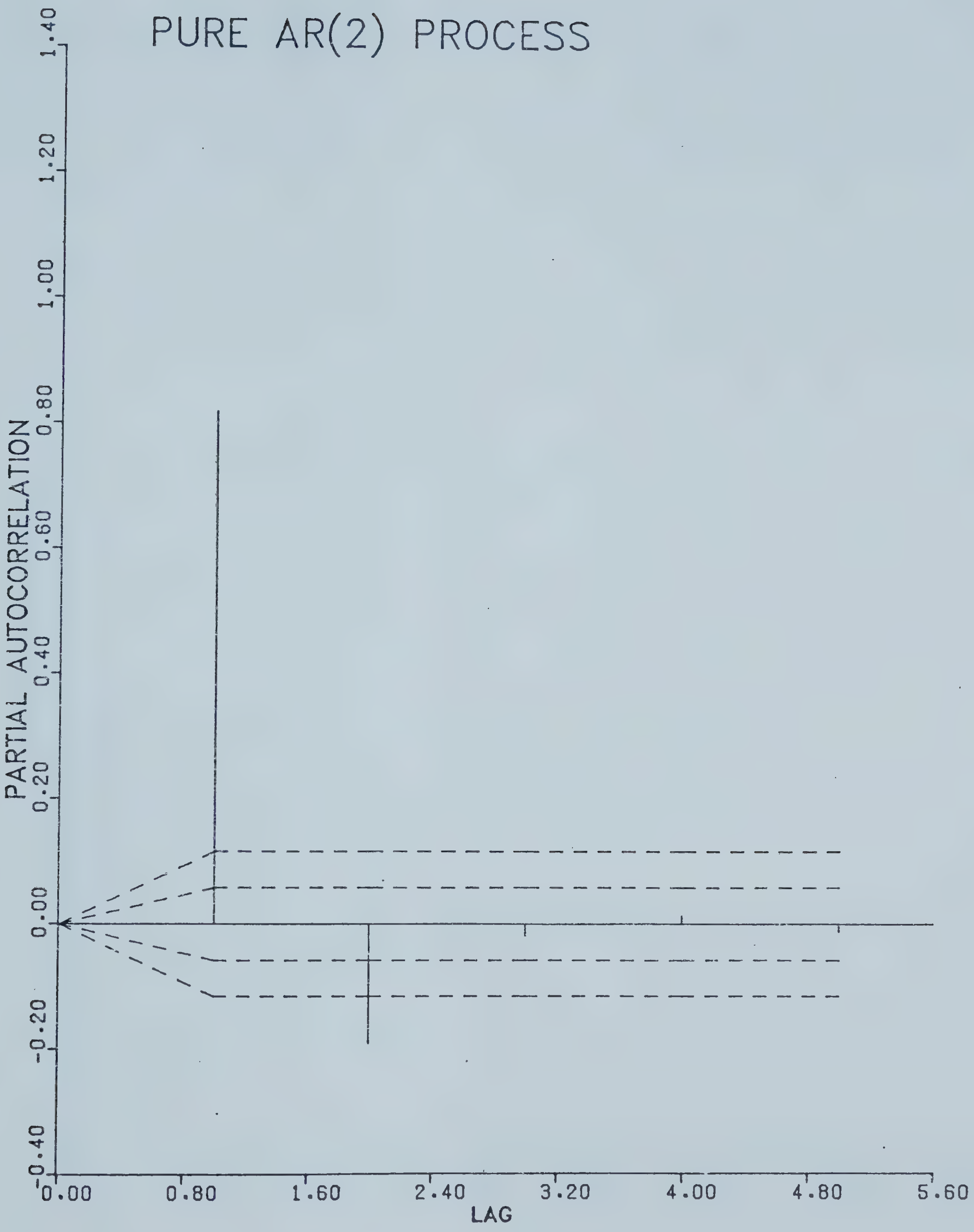

Figure 3.4 AR(2) Partial Autocorrelation

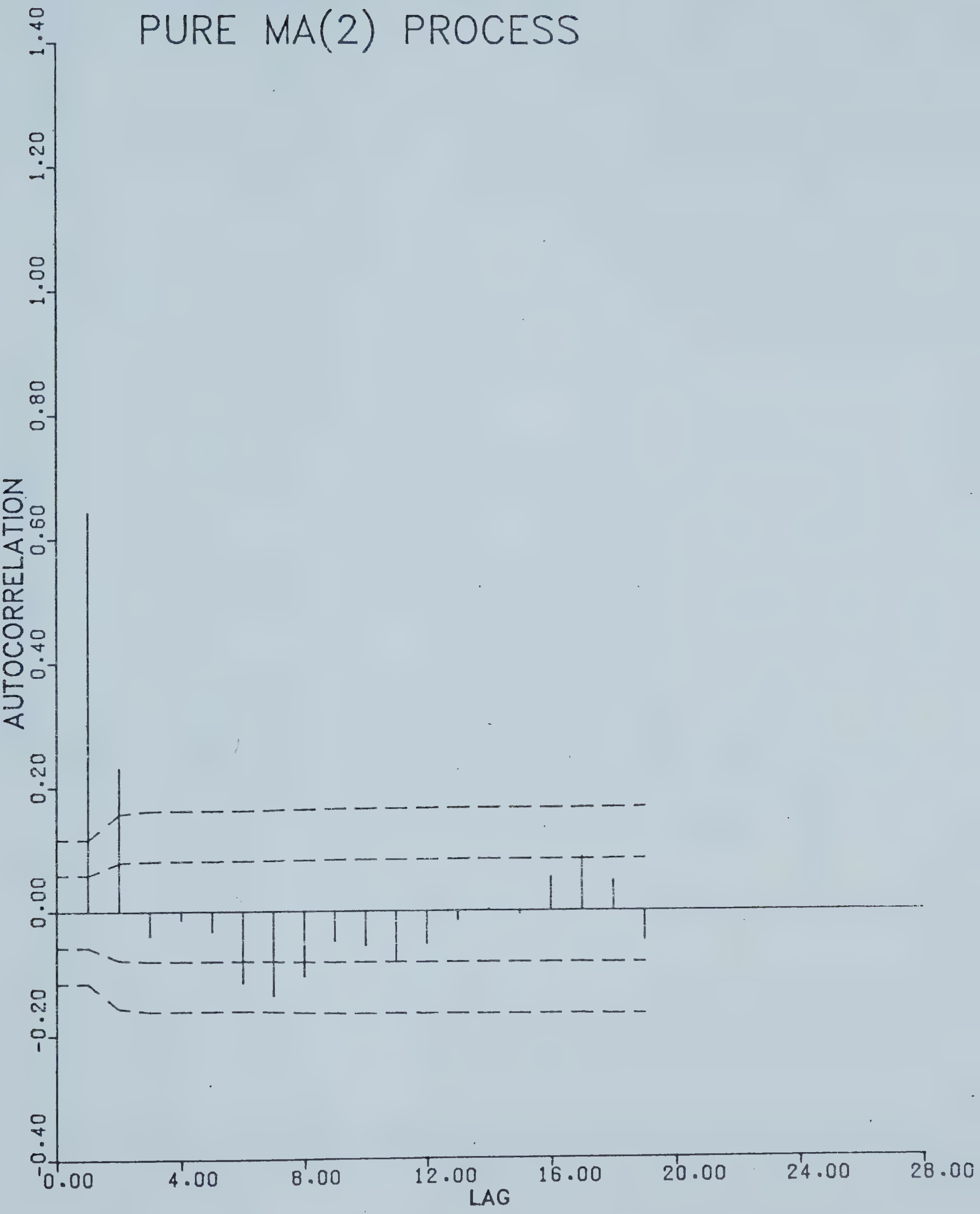

Figure 3.5 MA(2) Autocorrelation

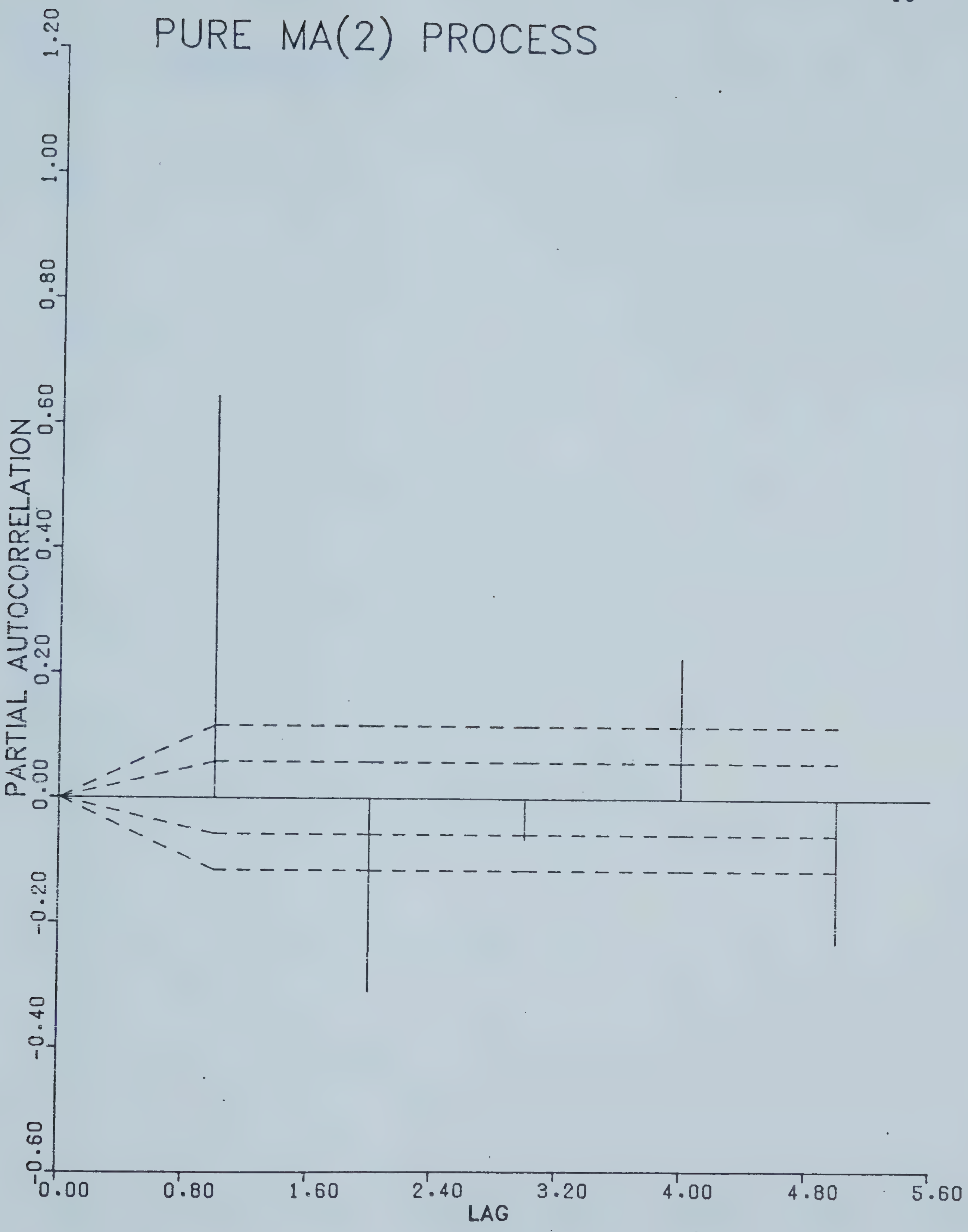

Figure 3.6 MA(2) Partial Autocorrelation

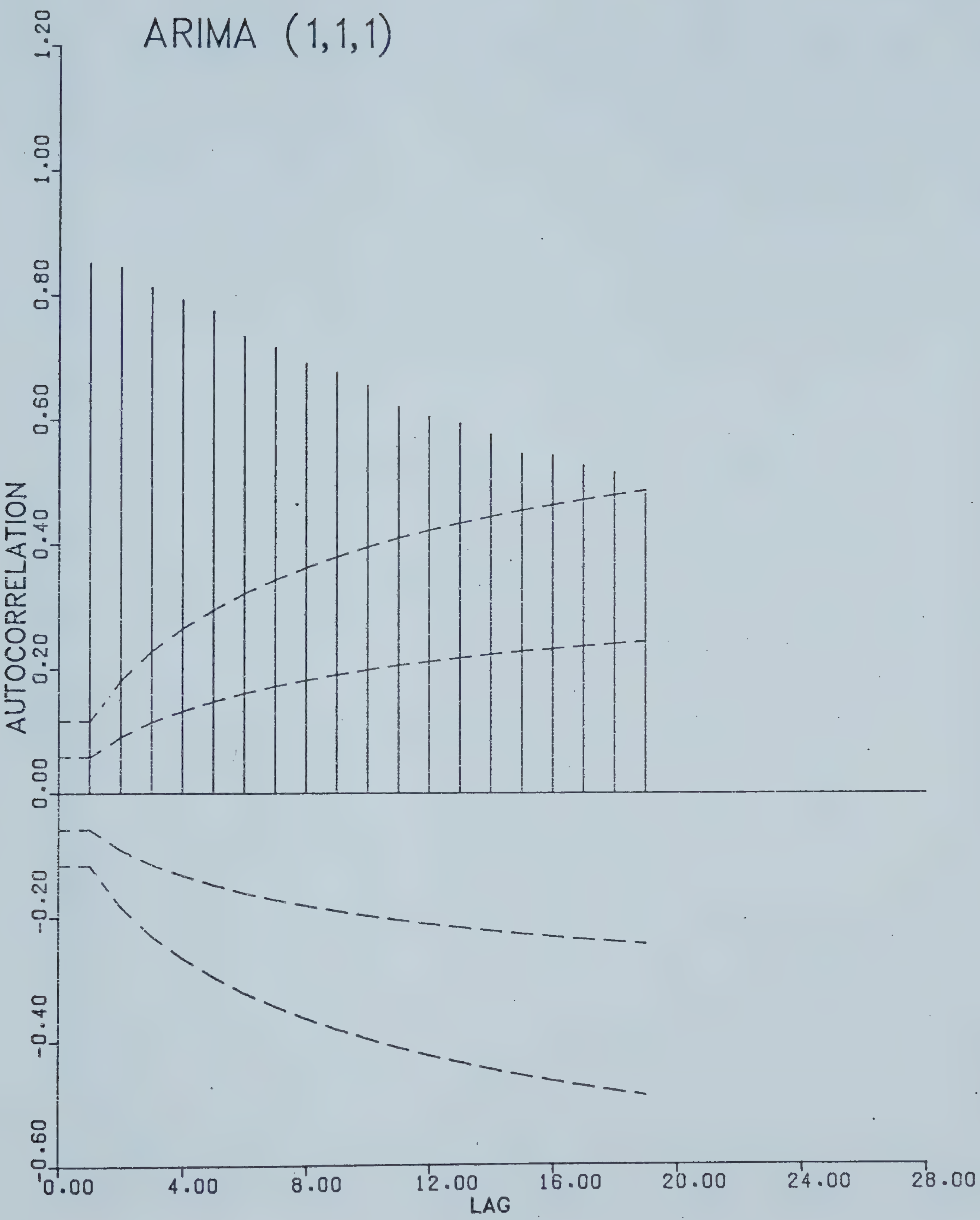

Figure 3.7 Autocorrelation of Simulated ARIMA(1,1,1)

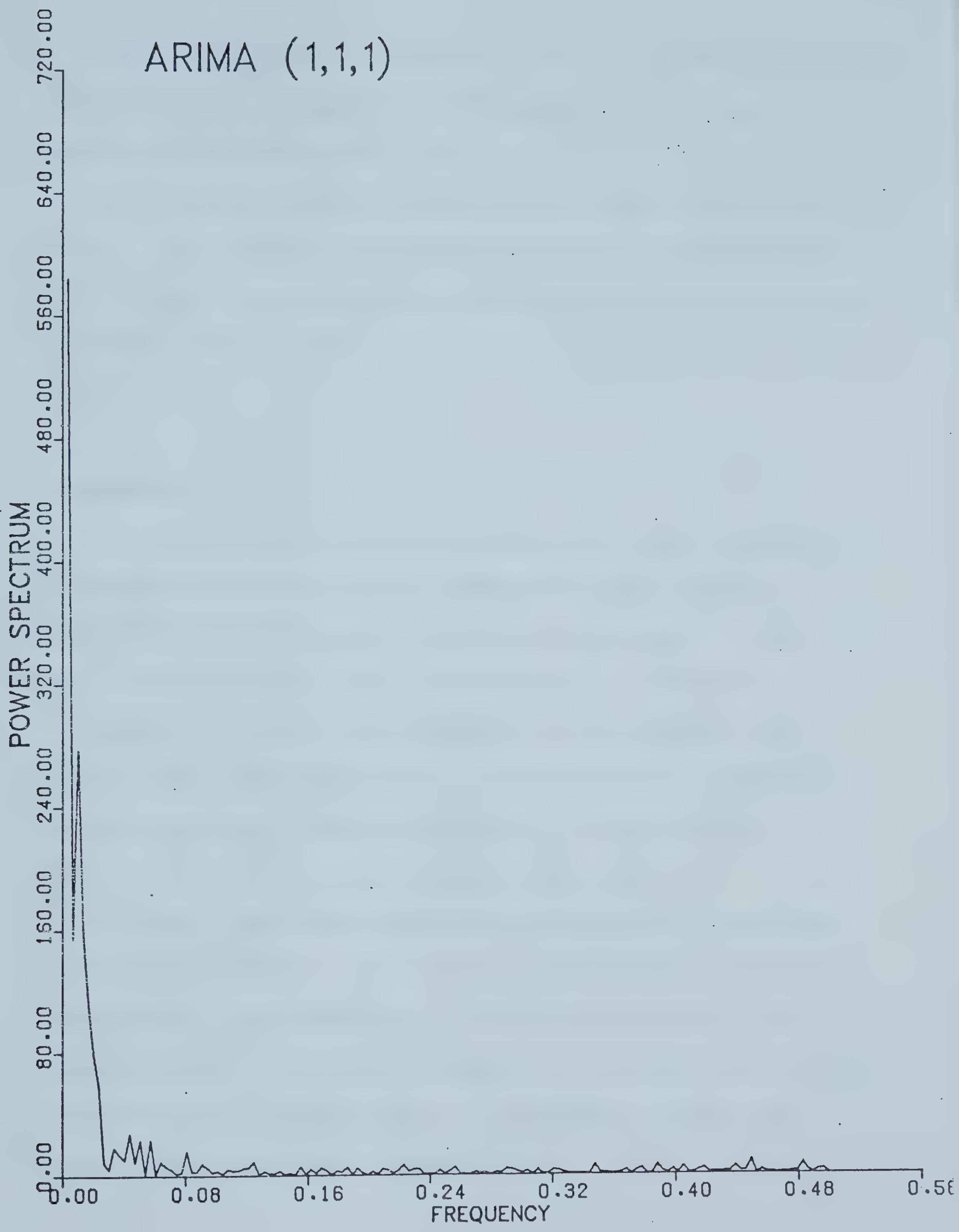

Figure 3.8 Power Spectrum of Simulated ARIMA(1,1,1)

After taking the first difference of the data, both the autocorrelation and partial autocorrelation die out quickly.(Figures 3.9 and 3.10).

This process would probably be initially identified as ARIMA(1,1,0), due to the behavior of the autocorrelation plot of the first difference. Diagnostics in the parameter estimation stage would later force an increase to ARIMA(1,1,1).

3.9 Summary

The main purpose of this chapter has been to develop and present examples of the autocorrelation, partial autocorrelation and power spectrum. These are the tools with which the structure of the noise model is identified.

Along with this, the concepts of stationarity and invertibility were presented. In the context of transfer function analysis, these correspond to the classical concepts of stability and minimum phase behavior.

But the techniques presented here must be developed further to be useful. To actually identify the noise model and estimate its parameters, the noise series must be available. This will only be possible if we have some means to partition our measurements of the plant output into deterministic and noise components.

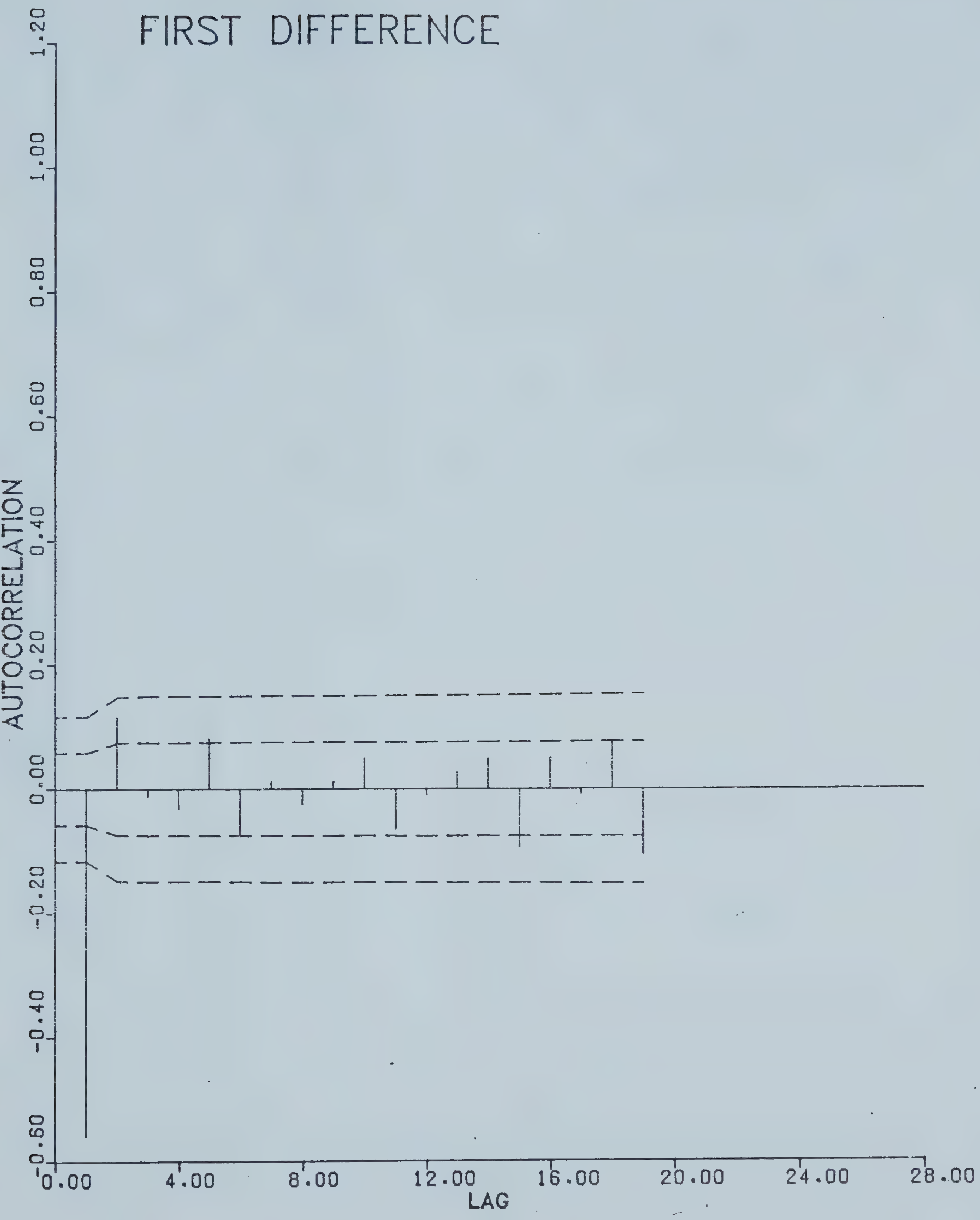

Figure 3.9 Autocorrelation of Differenced Data from

ARIMA(1,1,1)

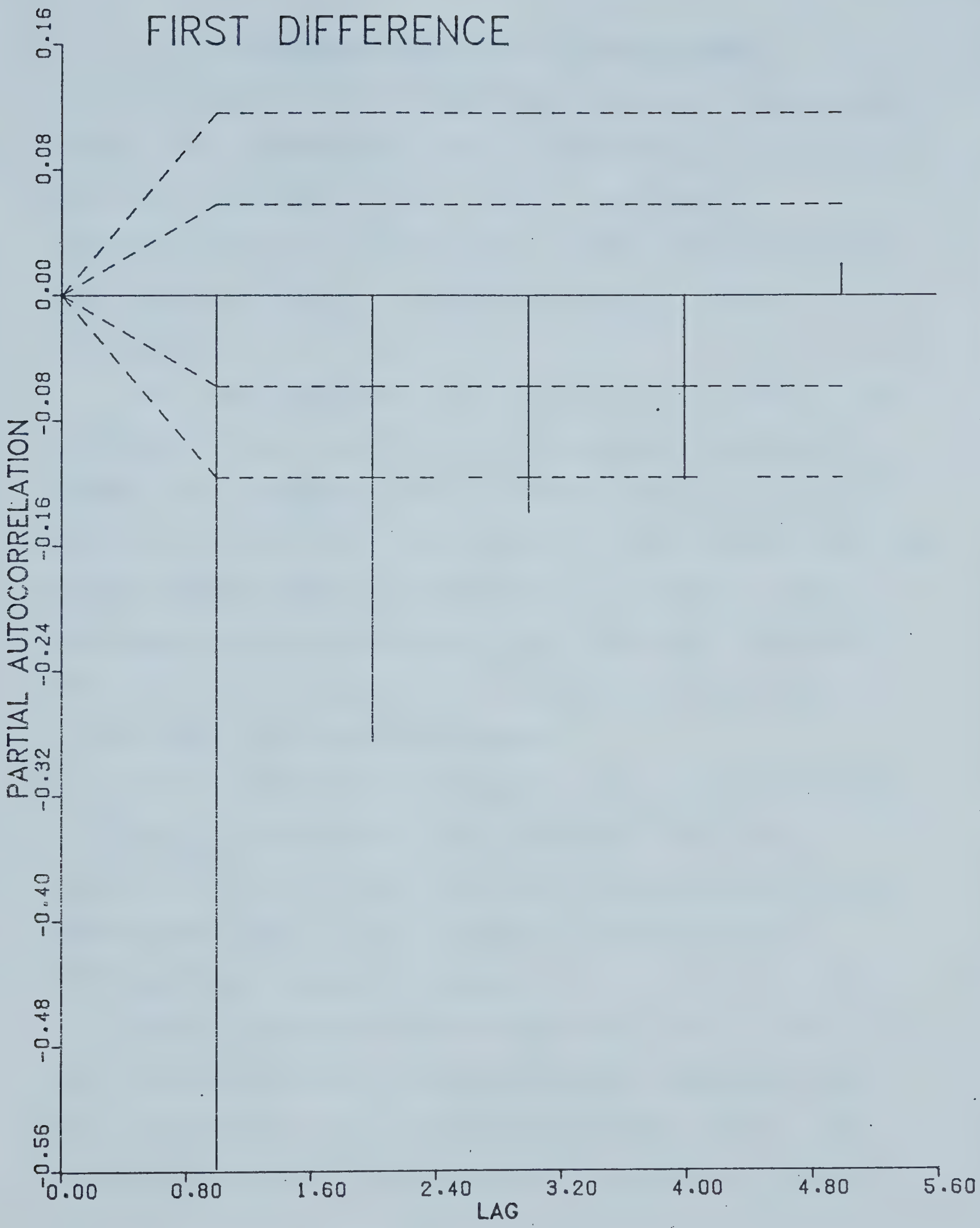

Figure 3.10 Partial Autocorrelation of Differenced Data from ARIMA(1,1,1)

4. TRANSFER FUNCTION PLUS NOISE MODELS

In this chapter, we will extend the results of the previous chapter. The fundamental tools of the correlation method have been introduced. First, we will consider a generalization of autocovariance, called cross-covariance. This function aids us in exploring apparent causal relationships.

The cross-covariance is of more utility, however, once we establish its connection to the impulse response of a system. This connection will be shown to be particularly direct when the input to the system is white noise. With the system impulse response available, we are able to partition our measurements into deterministic and noise components. This puts us into a position to identify both transfer function and noise model structure.

The last step is the simplest. Given a candidate model, we estimate parameters by least squares. Since this procedure can have trouble when starting, we first consider how to obtain good initial guesses. Then we examine nonlinear least squares in detail.

Lastly, once the parameter estimates are available, we must have some criteria for deciding their acceptability. This is covered in the section on diagnostic checks. To conclude the chapter, we present an illustrative example.

4.1 Cross-correlation

Recall the class of models being considered:

$$y(k) = \frac{\omega(z^{-1})}{\delta(z^{-1})} z^{-b} u(k) = n(k) \tag{4.1}$$

One idea intrinsic to this class of models is that u and y are causally related. In other words, we are interested in the conjoint variation of these two variables.

We define the cross-covariance from u to y as:

$$\gamma(u,y,j) = E[u(k)y(k+j)] \tag{4.2}$$

where both u and y denote deviations from the mean. (Note that the autocovariance of y is $\gamma(y,y,j)$.)

In general, $\gamma(u,y,j) \neq \gamma(y,u,j)$. But note:

$$\gamma(u,y,j) = E[u(k-j)y(k)] = E[y(k)u(k-j)] = \gamma(y,u,-j) \tag{4.3}$$

In a manner similar to autocorrelation:

$$\rho(u,y,j) = \frac{\gamma(u,y,j)}{\sigma(u)\sigma(y)} \qquad k=0,\pm 1,\ldots \tag{4.4}$$

defines the cross-correlation function. The cross-covariance is best estimated as:

$$c(u,y,j) = \begin{cases} (1/N)\Sigma u(k)y(k+j) & k=1,\ \ldots,\ N-j \quad j=0,1,\ldots \\ (1/N)\Sigma y(k)u(k-j) & k=1,\ \ldots,\ N+j \quad j=-1,-2,\ldots \end{cases} \tag{4.5}$$

To estimate the cross-correlation:

$$\rho(u,y,j) = \frac{c(u,y,j)}{\sqrt{c(u,u,0)}\ \sqrt{c(y,y,0)}} \tag{4.6}$$

As before, we will require a criterion for deciding whether a particular term in the cross-correlation function is significant. Bartlett (1955) shows that the approximate standard error of a cross-correlation estimate is:

$$\sigma^2(r(u,y,j)) \cong (N-j)^{-1}\Sigma[\ \rho(u,u,i)\rho(y,y,i)+\rho(u,y,j+i)\rho(u,y,j-i)$$

$$+\rho^2(u,y,i)\{\rho^2(u,y,i) + (1/2)\rho^2(u,u,i) + (1/2)\rho^2(y,y,i)\}$$
$$-2\rho(u,y,j)\{\rho(u,u,i)\rho(u,y,j+i) + \rho(u,y,-i)\rho(y,y,j+i)\}]$$
$$i = -\infty,\ \infty \quad (4.7)$$

If u and y are not cross-correlated, $\rho(u,y,i)=0$, so that all but the first term in Equation (4.7) are zero:

$$\sigma^2(r(u,y,j)) \cong (N-j)^{-1}\Sigma\ \rho(u,u,i)\rho(y,y,i) \quad i=-\infty,\ \infty \quad (4.8)$$

If u is white noise:

$$\rho(u,u,i) = 0 \quad i \neq 0 \quad (4.9)$$

and by definition:

$$\rho(u,u,0) = \rho(y,y,0) = 1 \quad (4.10)$$

So on the hypothesis that u and y are not cross-correlated, and u is white noise:

$$\sigma^2(r(u,y,j)) \cong (N-j)^{-1} \quad (4.11)$$

4.2 Input Prewhitening

Suppose that after differencing the original series d times:

$$y(k) = v(0)u(k) + v(1)u(k-1) + \ldots + n(k) \quad (4.12)$$

where the weights $\{v(i)\}$ are the system impulse response. Multiplying by $u(k-j)$, and taking expectations:

$$\gamma(u,y,j) = v(0)\gamma(u,u,j) + v(1)\gamma(u,u,j-1) + \ldots + \gamma(u,n,j) \quad (4.13)$$

Assuming that $u(k-j)$ is uncorrelated with $n(k)$ for all j:

$$\gamma(u,y,j) = v(0)\gamma(u,u,j) + v(1)\gamma(u,u,j-1) + \ldots \quad (4.14)$$

Beyond some point, the impulse response of the system will die out. Truncating Equation (4.14) at the point where the $v(i)$ are effectively zero, and then writing the system of equations from k=0 to k=K:

$$\gamma uy = \Gamma uu\ V \tag{4.15}$$

where:

$$\Gamma uu = \begin{bmatrix} \gamma(u,u,0) & \gamma(u,u,1) & \dots & \gamma(u,u,j) \\ \gamma(u,u,1) & \gamma(u,u,0) & \dots & \gamma(u,u,j-1) \\ & & \dots & \\ \gamma(u,u,j) & \gamma(u,u,j-1) & \dots & \gamma(u,u,0) \end{bmatrix}$$

$$\gamma uy = [\gamma(u,y,0)\ \dots\ \gamma(u,y,k)],\quad V = [v(0)\ \dots\ v(j)]$$

Now, by substituting estimates for $\gamma(u,u)$ and $\gamma(u,y)$, we can solve for the impulse weights. However, we can obtain the same results more simply. Suppose that we represent the input u(k) as a time series:

$$u(k) = (\theta_u(z^{-1})/\phi_u(z^{-1}))a(k) \qquad a(k) = N(0,\sigma^2(a) \tag{4.16}$$

And model the output y(k) with the same filter, but a different input:

$$y(k) = (\theta_u(z^{-1})/\phi_u(z^{-1}))\beta(k) \tag{4.17}$$

Substituting for u(k) and y(k) in Equation (4.12) from Equations (4.16) and (4.17):

$$\beta(k) = v(z^{-1})a(k) + e(k)$$

$$e(k) = (\phi_u(z^{-1})/\theta_u(z^{-1}))n(k) \tag{4.18}$$

Multiplying Equation (4.18) by $a(k-j)$, taking expectations, and assuming no cross-correlation between $a(k)$ and e(k):

$$\gamma(a,\beta,j) = v(j)\sigma^2(a) \tag{4.19}$$

which yields the estimate for the impulse response:

$$v(j) = \gamma(a,\beta,j)/\ \sigma^2(a) \tag{4.20}$$

This process of fitting a time series model to the input series, u(k), is called prewhitening. Obviously, if the input is white to start with, the impulse response is just a scaling of the cross-correlation.

4.3 Identification

Once the impulse response has been arrived at, we can use it to estimate the noise series as:

$$n(k) = y(k) - v(z^{-1})u(k) \qquad (4.21)$$

Study of the autocorrelation, partial autocorrelation and power spectrum will yield the noise model structure. We can also use the impulse response to identify the structure of the transfer function.

Recall the form of model being used:

$$y(k) = (\omega(z^{-1})/\delta(z^{-1}))z^{-b}u(k) \qquad (4.22)$$

where:

$$\omega(z^{-1}) = \omega(0) - \Sigma\omega(i)z^{-i} \quad i = 1, \ldots, s$$
$$\delta(z^{-1}) = 1 - \Sigma\delta(i)z^{-i} \quad i = 1, \ldots, r$$

and the definition of impulse response:

$$y(k) = v(z^{-1})u(k) \qquad (4.23)$$

Equating Equations (4.22) and (4,.23) we obtain:

$$\delta(z^{-1})v(z^{-1})u(k) = \omega(z^{-1})z^{-b}u(k) \qquad (4.24)$$

Equating coefficients of equal powers of z^{-1} in Equation (4.24):

1. $v(i) = 0 \quad i=0, \ldots, b-1$
2. $v(i) = \Sigma v(i-j)\delta(j) = -\omega(i) \quad j=1, \min(i,r), \; i=b, \ldots, b+s$
3. $v(i) = \Sigma v(i-j)\delta(j) = 0 \quad j=1, \min(i,r), \; i \geq b+s+1$

(4.25)

That is, the first b impulse response weights will be zero. And the weights v(i), i≥b+s+1 will follow the homogeneous r'th order difference equation with initial conditions v(i), i=b+s+1-r, ..., b+s. The intermediate sequence of weights is dictated by a sequence of inhomogeneous r'th order difference equations. In particular, v(b) is the first nonzero weight, so identification of b is straightforward.

The choice of r, which is normally limited to 0, 1, or 2, is less direct. The contrast in impulse response between processes of various orders is not always clear. Here, the step response weights are more easily interpreted.

Let V(i) denote the i'th step response weight. Then:

$$V(i) = \Sigma v(j) \ , \ j=0, \ldots, i \qquad (4.26)$$

Without numerator dynamics (i.e. s = 0), the distinction in step response is quite clear. (See Figure 4.1) Zero'th order processes respond completely at the first step. First order processes follow a simple exponential curve. At least second order dynamics will be necessary to explain anything more complex. (overshoot with oscillation, etc.)

The addition of numerator dynamics makes the issue less clear, by adding terms to the initial response. Zero'th order processes with numerator dynamics will show a linear increase up to full response. But it is very difficult to discern the presence of numerator dynamics in first or second order processes. By underfitting the model initially, and adding numerator dynamics only if the model is inadequate, satisfactory results will be obtained.

4.4 Preliminary Parameter Estimates

From the cross-correlation, we have an estimate of the impulse response:

$$y(k) = v(z^{-1})u(k) \qquad (4.27)$$

We wish to find a starting point for estimating the parameters in:

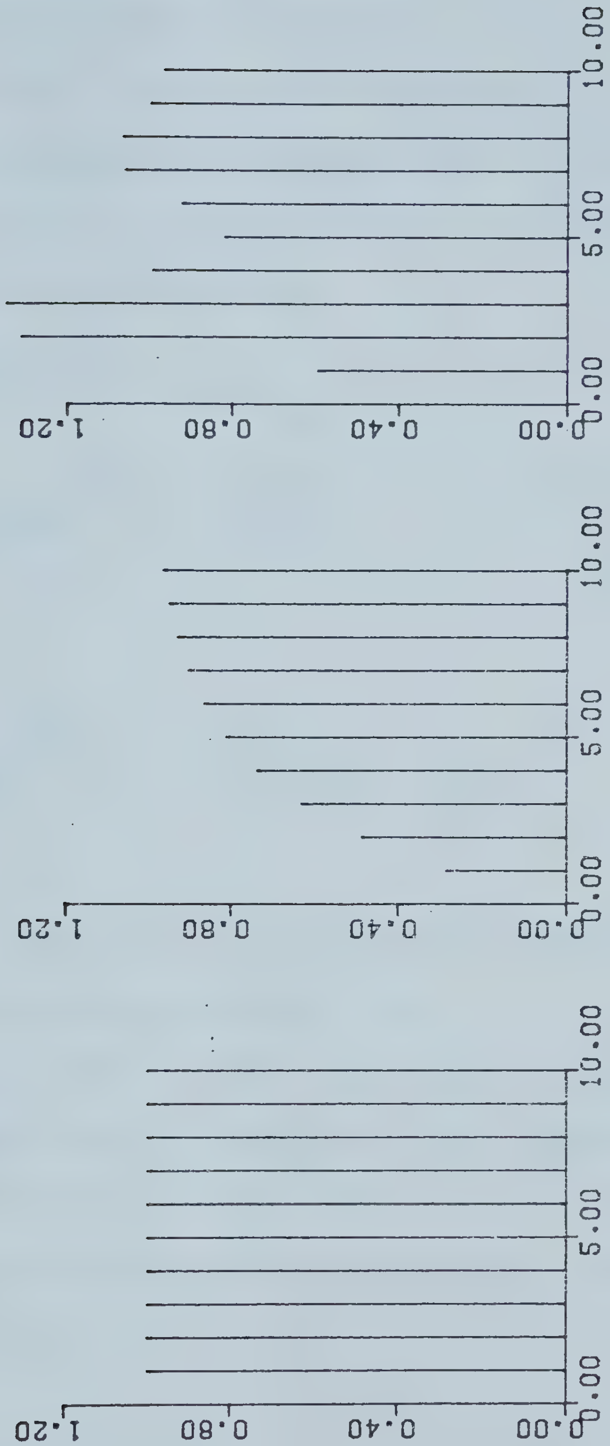

Figure 4.1 Representative Step Responses

$$y(k) = (\omega(z^{-1})/\delta(z^{-1}))z^{-b}u(k) \qquad (4.28)$$

Equating Equations (4.27) and (4.28):

$$\delta(z^{-1})v(z^{-1})u(k) = \omega(z^{-1})z^{-b}u(k) \qquad (4.29)$$

Expanding, grouping terms, and equating coefficients of equal powers of z^{-1} in Equation (4.29), we obtain the following preliminary estimates:

1. $v(j) = 0 \quad j<b$
2. If $r>0$, find $\delta(z^{-1})$ from: (4.30)

$$A\delta = V$$

where:

$\delta=[\delta(1) \ldots \delta(r)] \qquad V=[v(b+s+1) \ldots v(b++s+r)]$

$$[a_{ij}] = \begin{cases} v(b+s+i-j), & j\leq b+s+i \\ 0, & j>b+s+i \end{cases}$$

and matrix A is rxr.

3. $\omega(0) = v(b)$ (4.31)

4. If $s>0$, find $\omega(z^{-1})$ from:

   If $r>0$, $\omega=B\delta - v$ (4.32)

   $$\text{where } [b_{ij}] = \begin{cases} v(b+i-j), & j\leq i \\ 0, & j>i \end{cases}$$

   If $r=0$, $\omega = -v$ (4.33)

The noise model preliminary estimates are obtained as for time series models. (See Appendix A.)

It should be kept in mind that these estimates are extremely inefficient. In cases where the objective function (sum of squared errors) is very large at the starting point, it may be useful to start with all parameters set to a small, nonzero value (e.g. 10^{-3}).

4.5 Nonlinear Least Squares

In general terms, our problem is to minimize:

$$f(x) = Q^T(x,k)Q(x,k) \qquad (4.34)$$

where Q is a function that produces residuals at the

observation times, given the parameter vector x. The residuals are the difference between the model prediction based on parameters x, and the actual observation. f(x) is our objective function. The gradient is:

$$\nabla f = 2J^T Q \tag{4.35}$$

where J, the Jacobian, is:

$$J = \begin{bmatrix} (\partial Q/\partial x(1))|_1 & \ldots & (\partial Q/\partial x(m))|_1 \\ (\partial Q/\partial x(1))|_n & \ldots & (\partial Q/\partial x(m))|_n \end{bmatrix} \tag{4.36}$$

From this point on, let subscripts denote the stage of iteration. Approximate Equation (4.35) as:

$$\nabla f_{i+1} \cong 2J_i^T Q_{i+1} \tag{4.37}$$

and approximate Q_{i+1} by the Taylor series:

$$Q_{i+1} \cong Q_i + J_i(x_{i+1} - x_i) \tag{4.38}$$

Substituting Equation (4.38) into (4.37):

$$\nabla f_{i+1} \cong 2J_i^T J_i(x_{i+1} - x_i) + 2J_i^T Q_i \tag{4.39}$$

At the minimum, a necessary condition is:

$$\nabla f_{i+1} = 0 \tag{4.40}$$

Substituting Equation (4.40) into (4.39):

$$x_{i+1} = x_i - \{J_i^T J_i\}^{-1} J_i^T Q_i \tag{4.41}$$

which is Gauss' method of least squares.

4.5.1 Levenburg - Marquardt correction

To ensure that the matrix inversion required by Equation (4.41) is possible, it is sufficient that the matrix $J^T J$ be positive definite. Scale $J^T J$ as:

$$\Pi = C^{-1} J^T J C^{-1} \tag{4.42}$$

where:

$$[c_{ij}] = \begin{cases} \sqrt{|J^TJ|_{ij}} & , i=j \\ 0 & , i \neq j \end{cases}$$

Then:

$$[J^TJ]^{-1} = C^{-1}\Pi^{-1}C^{-1} \tag{4.43}$$

Positive definiteness can be guaranteed if we let:

$$[J^TJ]^{-1} = C^{-1}[\Pi + \lambda I]^{-1}C^{-1}$$

$$[J^TJ]^{-1} = [J^TJ + \lambda C^2]^{-1} \tag{4.44}$$

where λ is a positive constant such that $\lambda > -\min\{a_i\}$. Here, the a_i are the eigenvalues of Π. That is, λ guarantees invertibility by moving the eigenvalues of J^TJ into the right half plane. Substituting Equation (4.44) into (4.41):

$$x_{i+1} = x_i - [J_i^TJ_i + \lambda\ C_i^2]^{-1}J_i^TQ_i \tag{4.45}$$

We can further stabilize the algorithm by choosing:

$$x_{i+1} = x_i - C^{-1}{}_i[C_i^{-1}J_i^T J_i C_i^{-1} + \lambda I]^{-1}C_i^{-1}J_i^TQ_i \tag{4.46}$$

As we increase λ, λC^2 dominates J^TJ, and the procedure looks more like steepest descent:

$$x_{i+1} = x_i - (1/2\lambda)C_i^{-2}\nabla\ f_i \tag{4.47}$$

But also note that increasing λ decreases the step size. As the minimum is approached, λ should approach zero, to return us to Gauss' method. Thus, let:

$$\lambda_{i+1} = \lambda_i/\nu \tag{4.48}$$

where ν is a constant greater than 1. For the transfer function plus noise problem, the residuals a(k) are calculated in three steps:

1. $y'(k) = (\omega(z^{-1})/\delta(z^{-1}))z^{-b}u(k)$ (4.49)
2. $n(k) = y(k) - y'(k)$ (4.50)
3. $a(k) = (\phi(z^{-1})/\theta(z^{-1}))n(k)$ (4.51)

The algorithm will become unstable if there are redundant parameters. A redundant parameter will result in one column of the Jacobian being linearly dependent on the others. Thus, the matrix will become singular, and cannot be inverted.

4.6 Diagnostic Checks

Once a particular model has been fitted, its adequacy must be checked. Most diagnostics are based on the model residuals. The following five checks should be performed:

1. The input, $u(k)$, should not be cross-correlated with the residuals. If it is, there is a "residual" relationship between input and output which has not been explained by the model.
2. The model residuals should not be autocorrelated. If the residuals are autocorrelated, but not cross-correlated with the output, $y(k)$, then there is some difficulty in the noise model which induces this auotcorrelation.
3. We can also test the first few terms of the cross-correlation, $r(\alpha,a,k)$, or the autocorrelation, $r(a,a,k)$. This will be a chi-square test, where:

$$\chi^2(\nu) = \nu s^2/\sigma^2 \ , \ E[\chi^2(\nu)] = \nu \qquad (4.52)$$

and:

ν = number of degrees of freedom
s^2 = observed variance
σ^2 = true variance

a. The statistic:

$$S = N\sum_{i=0,\ \ldots,\ j} r^2(\alpha,a,i) \ , \ N=(n-\max(s+b+p,p')) \qquad (4.53)$$

will be distributed as $\chi^2(j-(r+s))$, where:

n = number of observations

p' = prewhitening transform autoregressive degree

j = number of cross-correlations to be considered

b. The statistic:

$$Q = N\Sigma r^2(a,a,i) \ , \ N = (n-(s+b+p)) \qquad (4.54)$$

will be distributed as $\chi^2(j-(p+q))$.

If either statistic is much larger than its expected value, the corresponding correlation ($r(\alpha,a,k)$ or $r(a,a,k)$) should be viewed with suspicion.

4. The uncertainty interval for a parameter should not include zero.

5. The power spectrum of the residuals should be white.

If all these checks are passed, the model can be considered a good candidate. Given more than one candidate model, that with fewest parameters should be chosen.

4.7 Stirred Tank Heater

As an example, we will consider modelling a stirred tank heater. (See Figure 4.2) Our objective is to find the transfer function plus noise model for outlet temperature response to steam flow.

To obtain the input-output data, an open-loop test must be performed. This requires that we perturb the input, and sample the plant output.

A priori, it is difficult to define an optimum input signal (Box and Jenkins,(1976)). The basic criterion is that

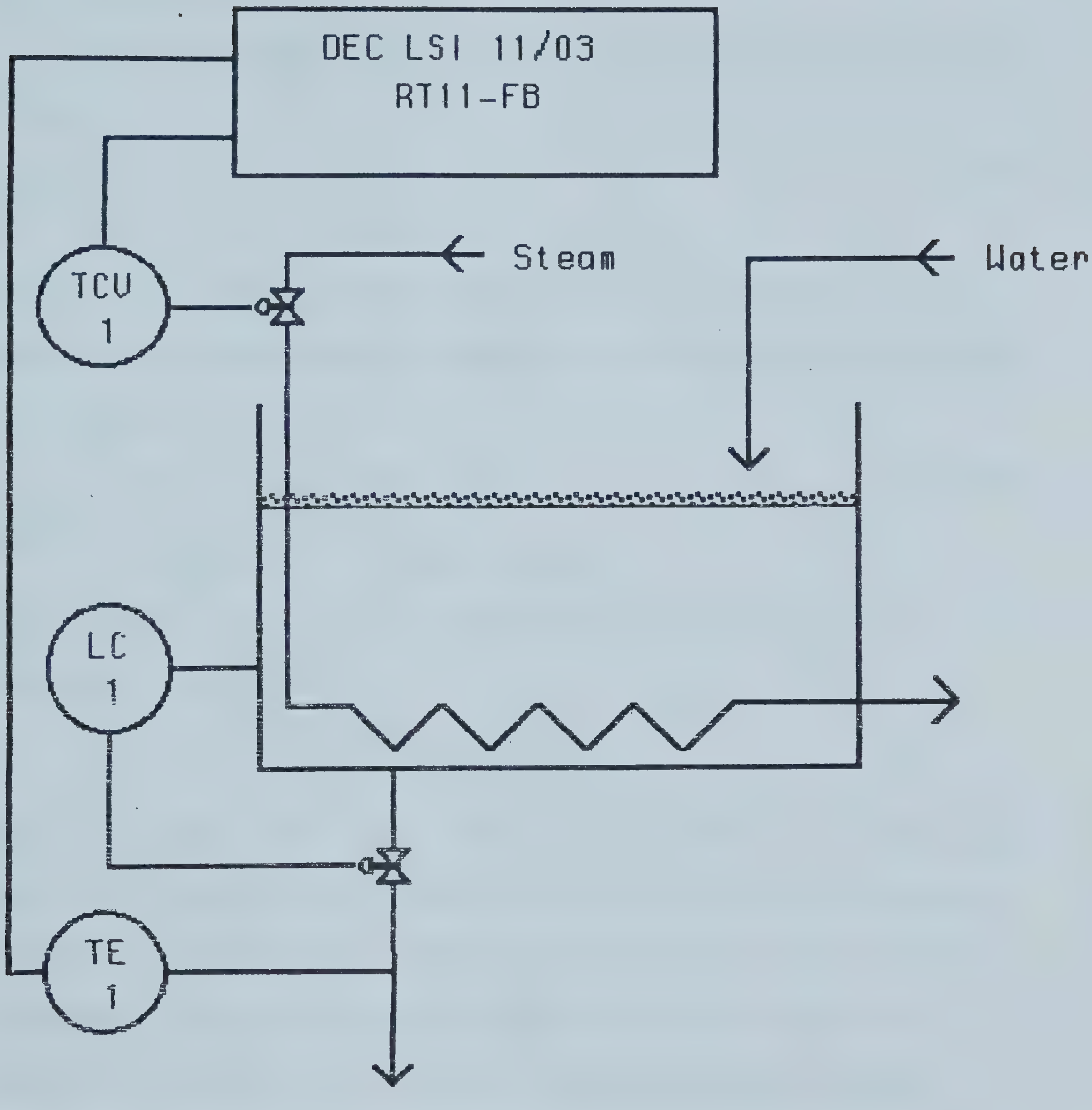

Figure 4.2 Stirred Tank Heater

it must be rich enough to excite all the modes of interest. This criterion is satisfied by a white noise sequence. The most common white noise generator is the central limit theorem generator.

Approximately normal random variables can be generated from:

$$p = n_1 + \ldots + n_{12} \qquad (4.55)$$

where:

$$\sigma^2(p) = 1 \ , \ p = 6$$

and n is uniformly distributed in [0,1]. Uniform distributions are usually achieved by congruential schemes. For example,

$$n_{i+1} = cn_i (\text{modulo } m) \qquad (4.56)$$

where: n_0 is odd $\quad m=2^d+1$
$c = 8t\pm3$ $\quad$ t some integer

will yield 2^{d-2} values in the range [0, m-1] before repeating. We could use:

$$c = 65539 = 8*8192 + 3$$
$$m = 2^{31} + 1$$

Given an input signal, we must also decide on the sampling rate, and sample size. Sampling rate is determined by the need to recognize high frequency components. The highest frequency that can be recognized is determined by the sampling theorem to be one half the sampling frequency. Sample size is determined by the need to recognize low frequency components. As a rule of thumb, estimates of lag components of more than 20% - 30% of the data should probably be avoided. The least constraining choice is to sample as quickly as possible for as long as possible, while

acknowledging these caveats:

1. Very large data sets make statistical inferences meaningless because of the explosion of degrees of freedom.
2. The variance of a parameter estimate is roughly proportional to the inverse square root of the number of samples.
3. Data collection can be a very expensive process.

In the present example, a central limit theorem generator was used to build up a steam valve position input with mean 50% and variance 20%. The sampling interval selected was 5 seconds (0.2 Hz). A total of 200 points were gathered. (See Appendix B for a listing of the data.) This scheme is probably useful for frequencies from 0.01 Hz to 0.1 Hz. The test results are presented in Figures 4.3 - 4.6.

Firstly, the cross-correlation (Figure 4.3) appears reasonable, in that an increase in steam flow is correlated with an increase in temperature. Note that the cross-correlation at lag 1 is just significant, so that $b = 1$.

The step response (Figure 4.4) shows a process with overshoot, so that at least second order dynamics are required.(i.e. $r = 2$) No guess as to numerator dynamics can be made at this point. The autocorrelation of the noise estimate (Figure 4.5) dies out rather slowly. Inspecting the noise partial autocorrelation (Figure 4.6), it appears we have a largely autoregressive process ($p = 1$), but perhaps

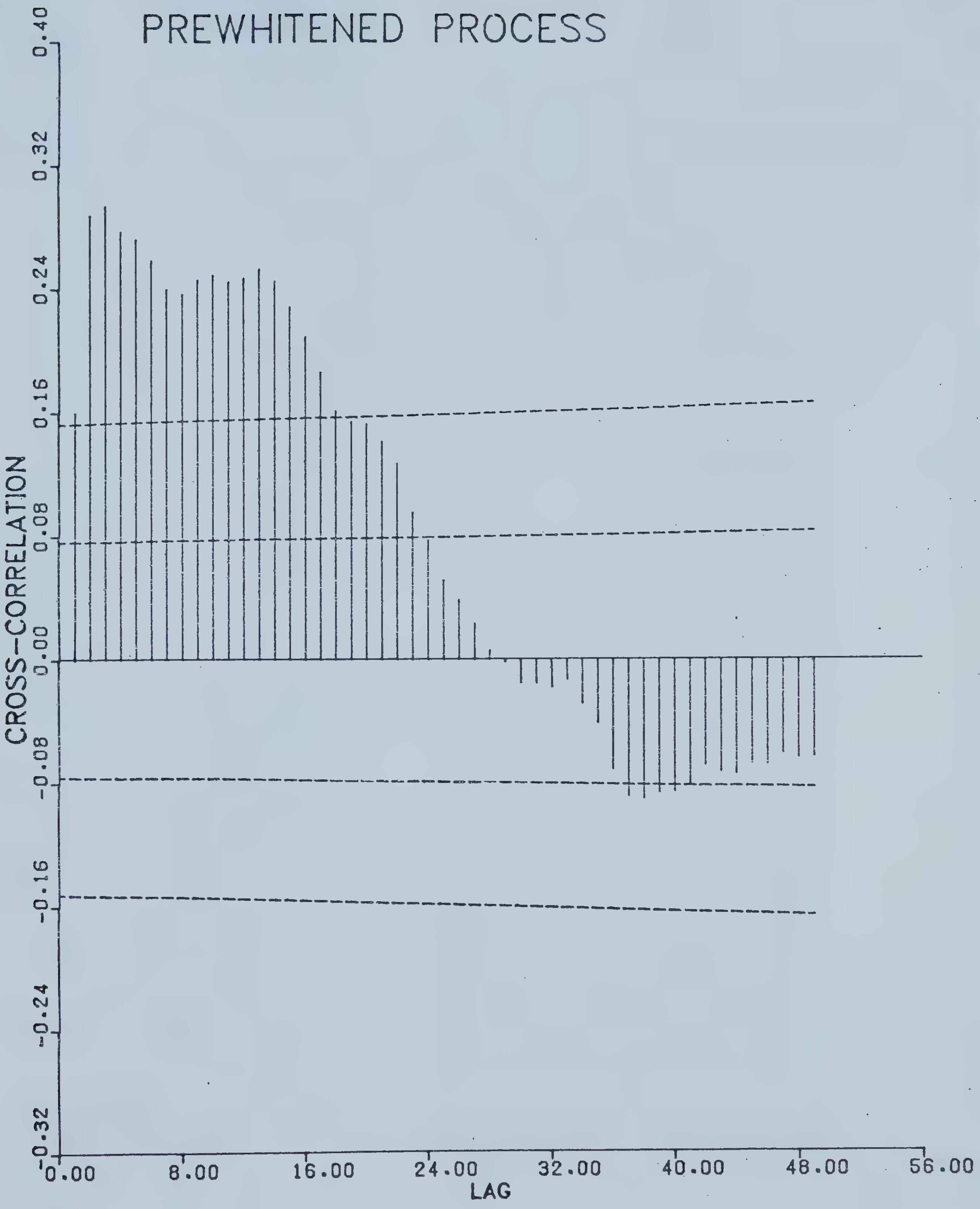

Figure 4.3 Process Cross-correlation

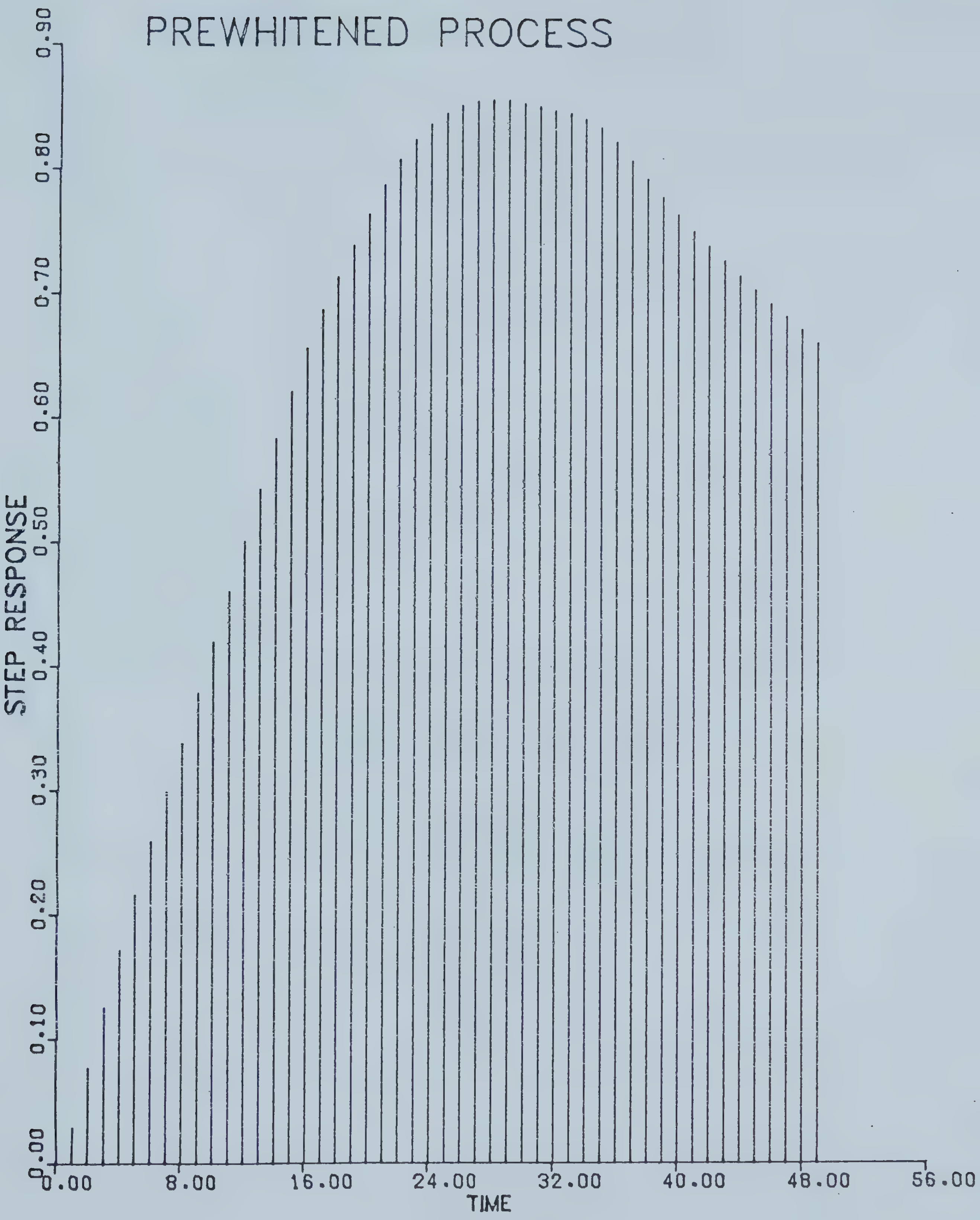

Figure 4.4 Step Response

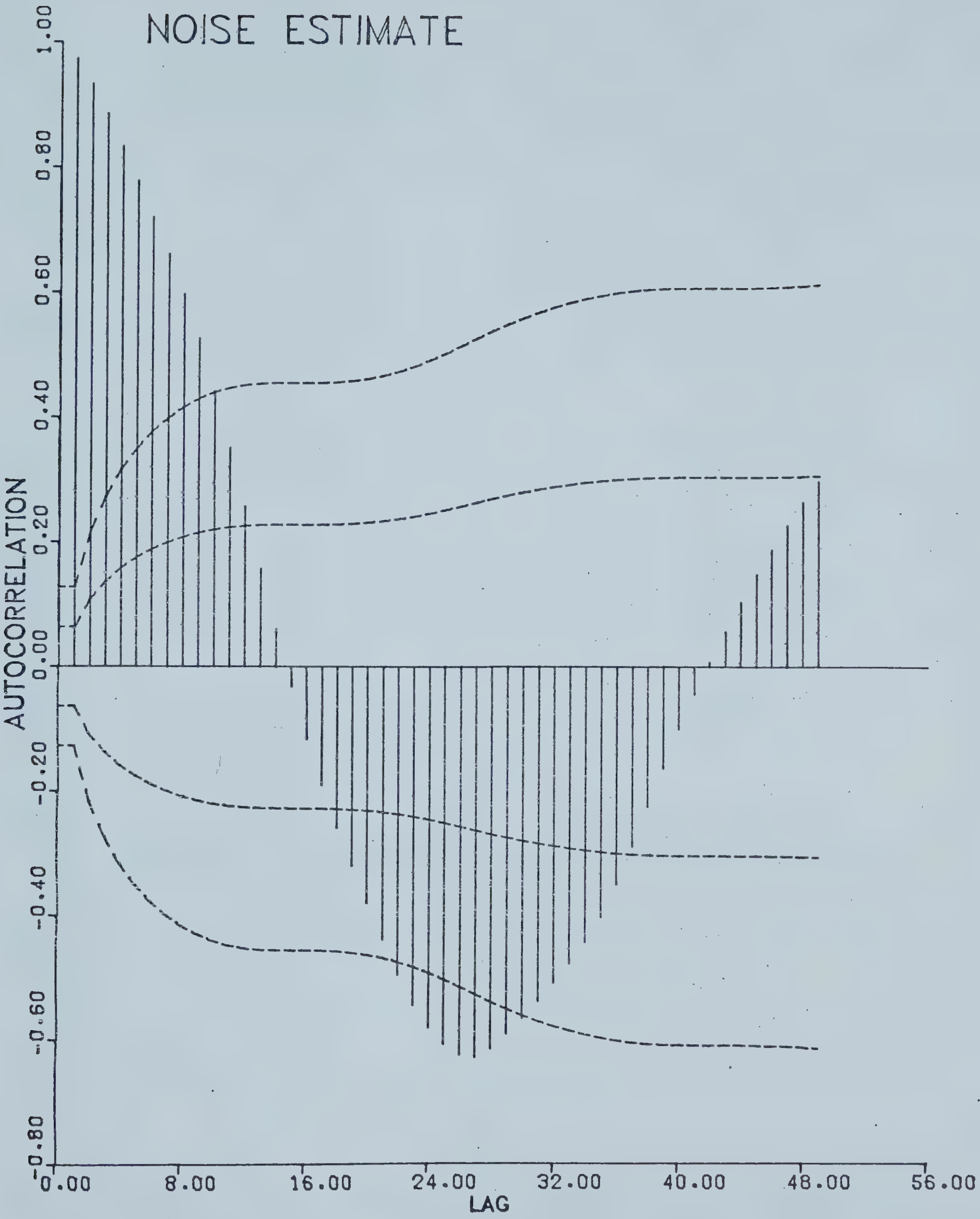

Figure 4.5 Noise Autocorrelation

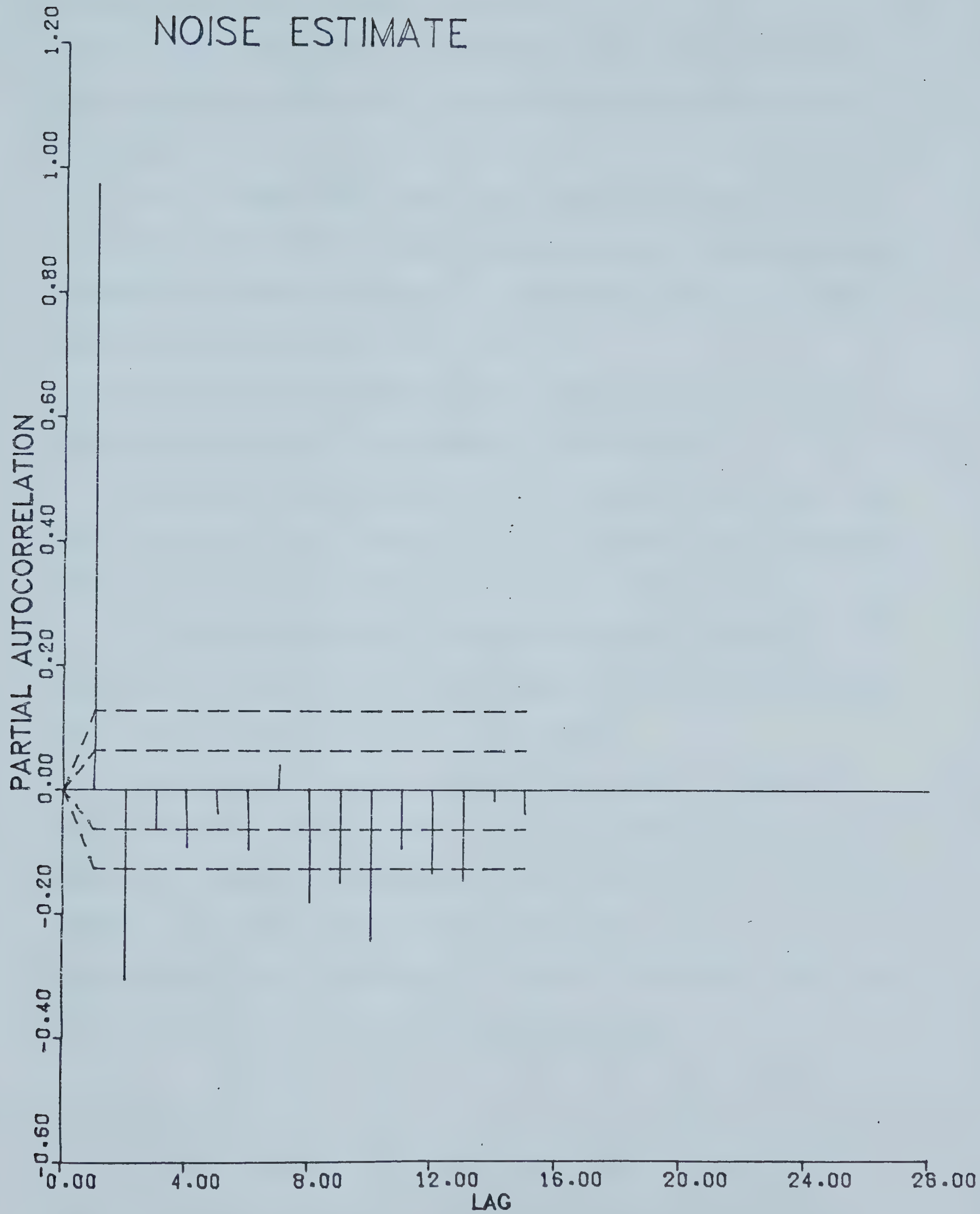

Figure 4.6 Noise Partial Autocorrelation

with some moving average character.

In this case, the tentative transfer function plus noise model has orders of (r,s,b) - (p,d,q) equal to (2,0,1) - (1,0,0).

We find eventually that the diagnostic checks are satisfied only with the addition of numerator dynamics, plus one moving average parameter in the noise model. The best model is of orders (2,1,1) - (1,0,1).

The plots of parameter value versus iteration number (Figures 4.7 and 4.8) show smooth convergence.

The autocorrelation plot of the residuals (Figure 4.9) shows no significant terms. And the residual power spectrum (Figure 4.10) lies within the bounds for white noise.

The cross-correlation between input and residuals (Figure 4.11) shows one significant term, but this is at a very large lag, so it can be discounted.

The parameter values obtained are given in Table 4.1. Thus, the model for this case is fairly straightforward to obtain. It should be emphasized that even for this problem, building the model required an iteration, from identification and estimation, through diagnostic checking and correction, thence back to estimation.

4.8 Summary

In this chapter, our first step was to define the cross-correlation function. Both the cross-correlation function and impulse response are nonparametric models of a

system. Perhaps, then, it is not surprising that the two are closely related. In the simplest case of white noise input to a system, the impulse response is just a scaling of the cross-correlation. Even when the input is not white, there is an orthogonal set of equations relating cross-correlation to impulse response.

	δ_1	δ_2	ω_0	ω_1	ϕ_1	θ_1
Value	1.01	-0.0064	0.0246	-0.0218	0.956	0.08
$\pm 2\sigma$	0.01	0.011	0.00002	0.0003	0.002	0.03

Table 4.1 Results of Parameter Estimation

This relationship is important, since we can determine the cross-correlation function from experimental data. Thus, we can estimate the impulse response. Finally, from the impulse response, we can identify the structure of the transfer function.

With both the transfer function and noise model identified, we can attempt to estimate a set of parameters. Before doing so, we may want to generate a set of preliminary estimates as a starting point for the least squares routine.

With the parameter estimates in hand, we run through a series of diagnostic checks. If all checks are passed, we have a good candidate model. If the checks are not passed, we modify the model structure accordingly, and estimate a new parameter set.

In developing the transfer function plus noise model, we go through an alternating series of steps. On one hand,

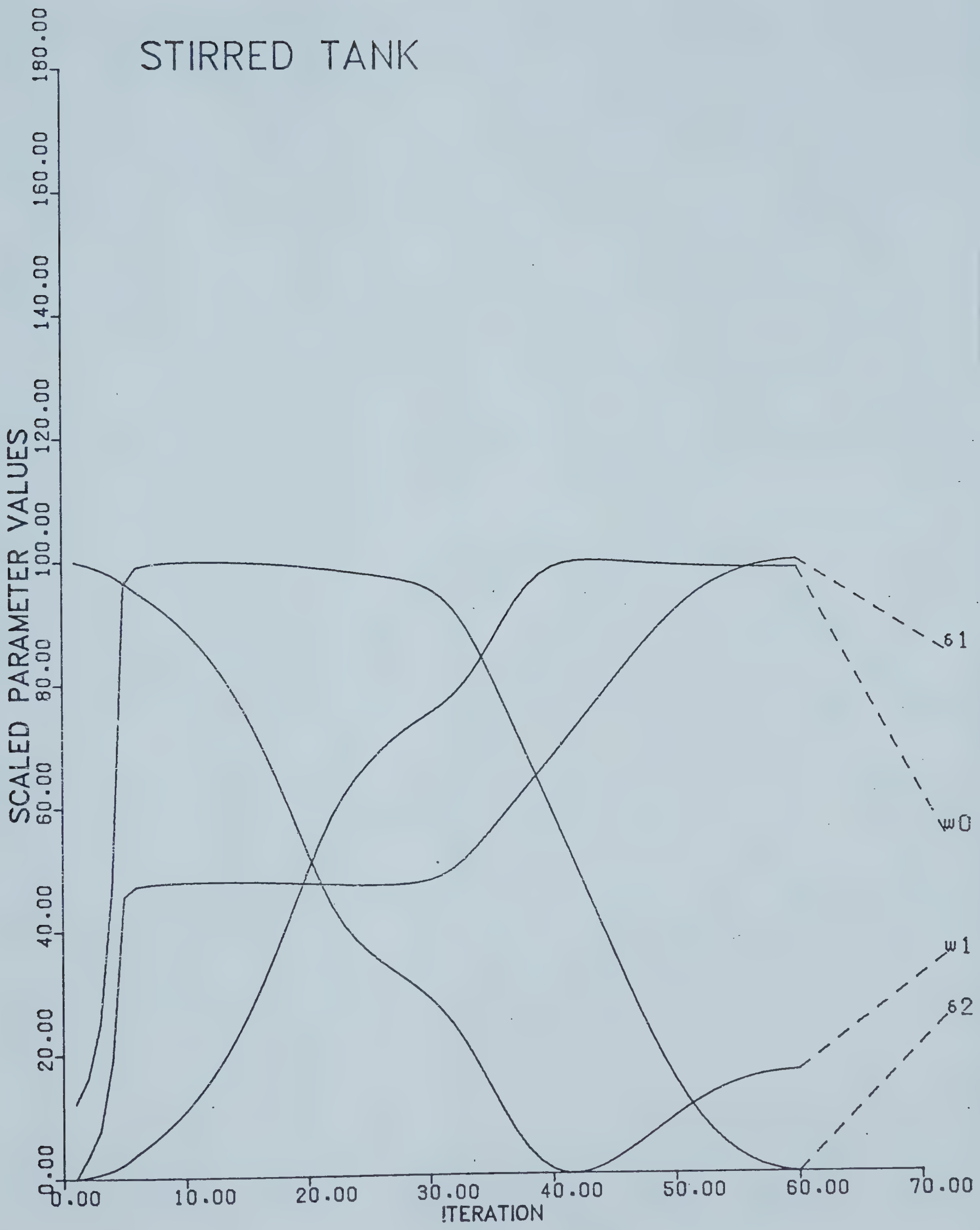

Figure 4.7 Fitting of Transfer Function Parameters

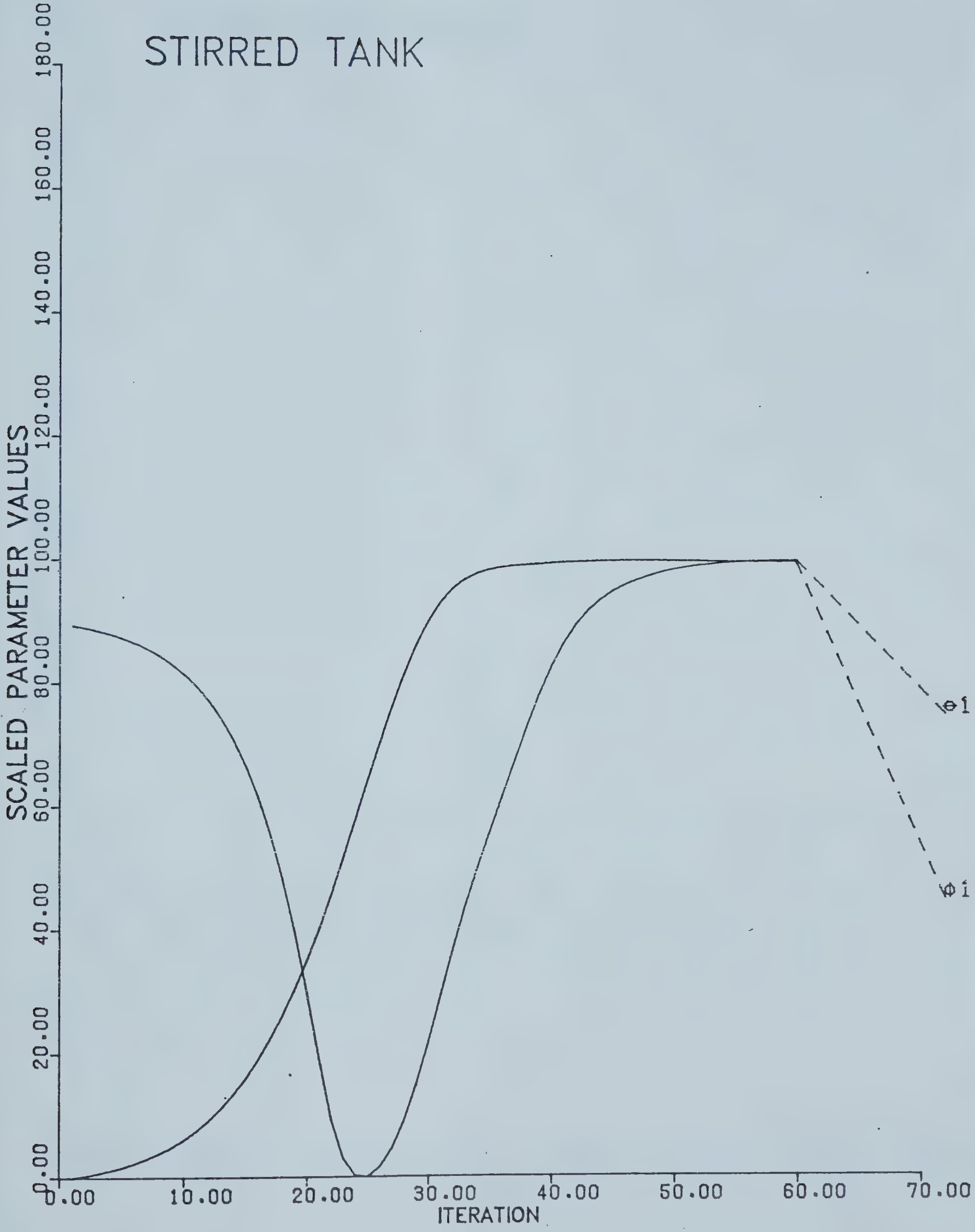

Figure 4.8 Fitting of Noise Model Parameters

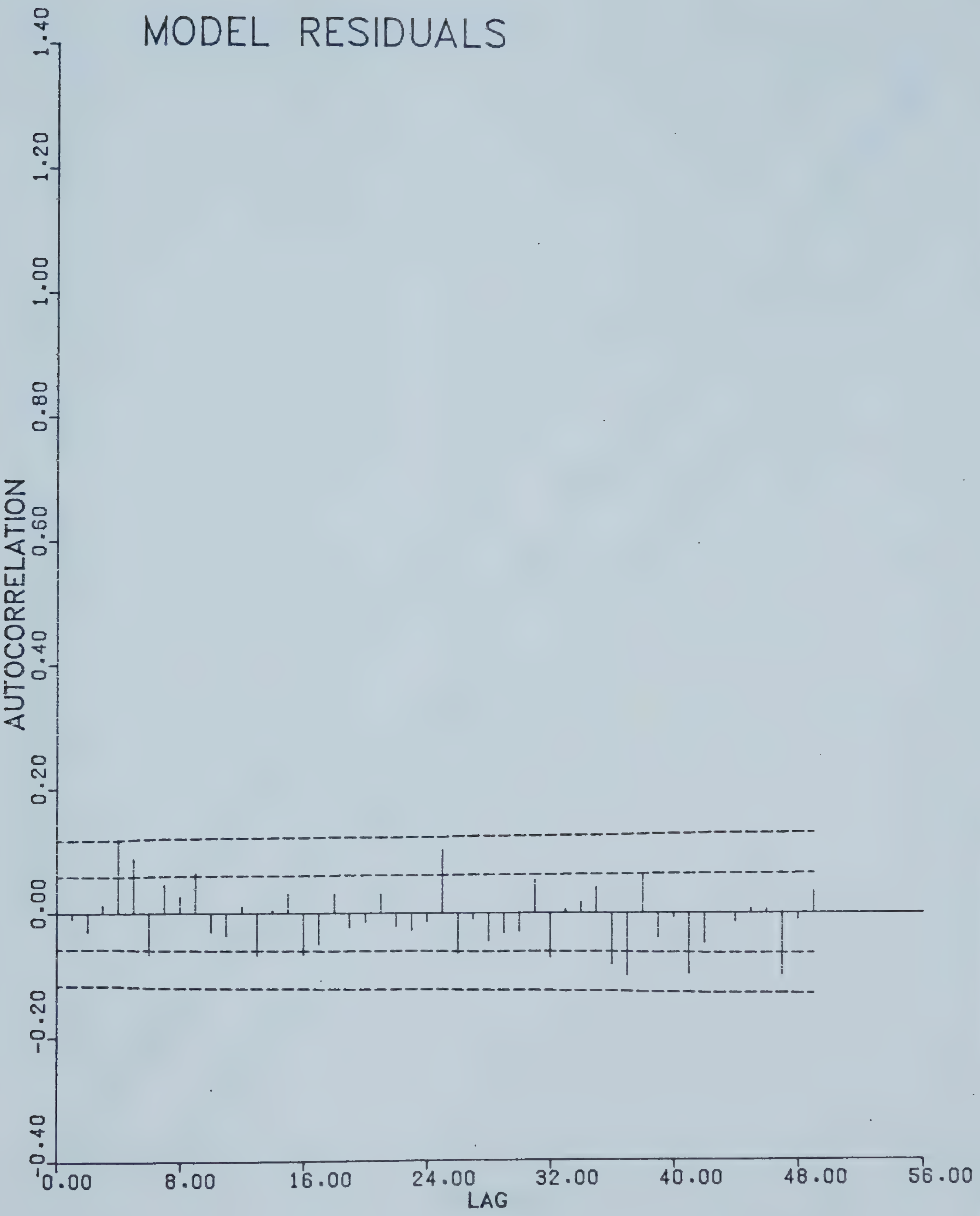

Figure 4.9 Residual Autocorrelation

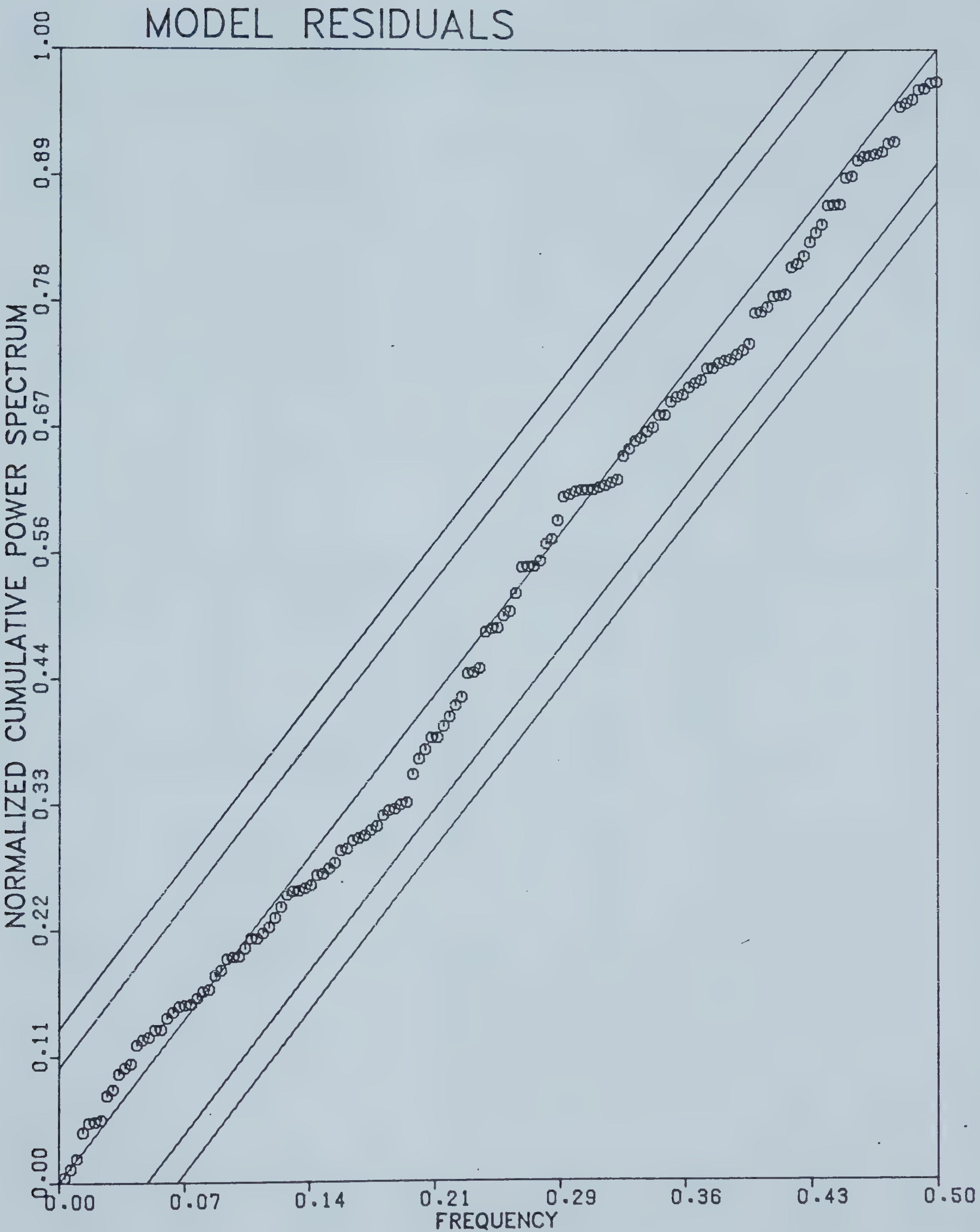

Figure 4.10 Residual Cumulative Spectrum

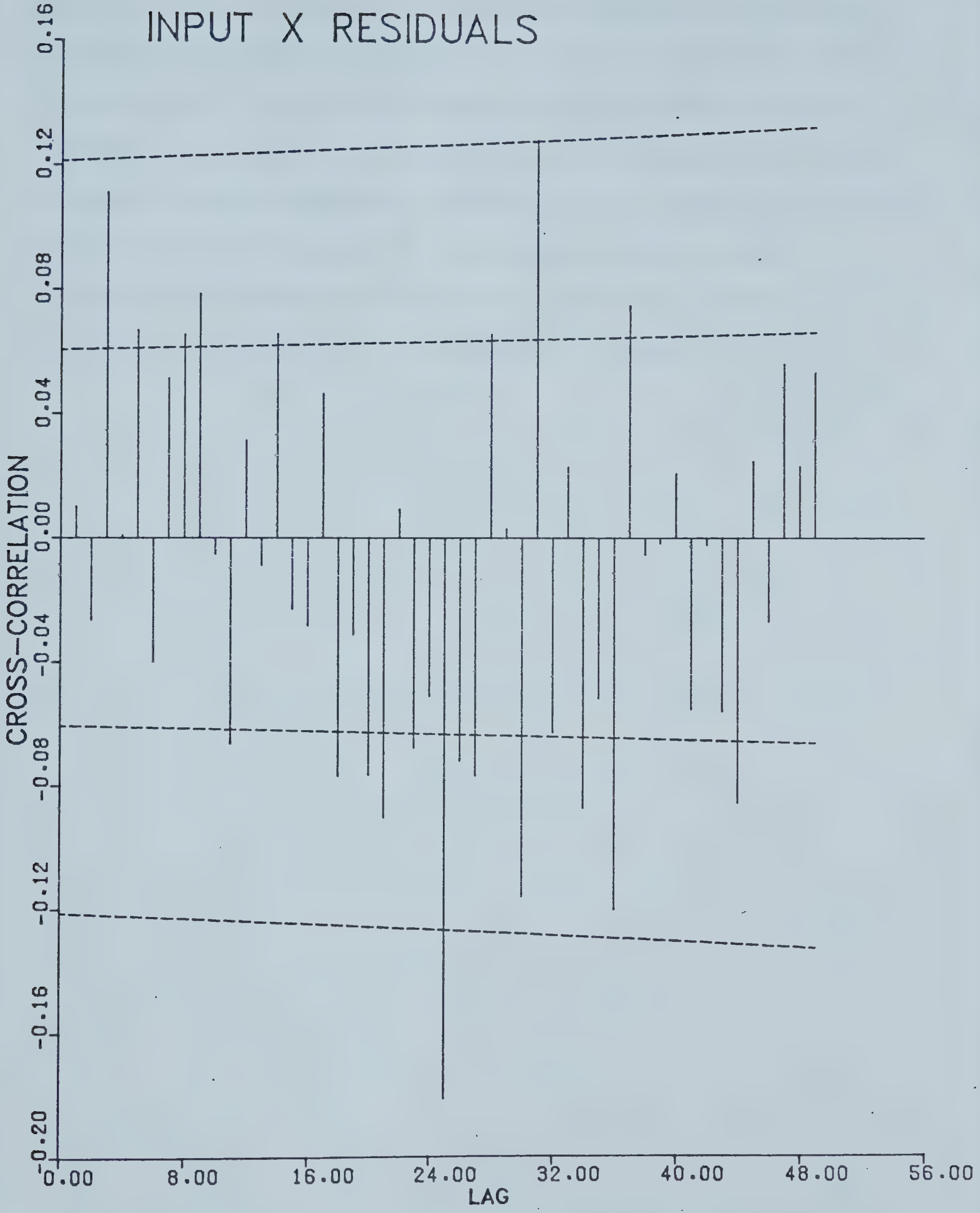

Figure 4.11 Residual Cross-correlation with Input

we have a set of strictly analytical procedures(calculate and display autocorrelation, etc.). These steps can easily be automated. On the other hand, we have a set of pattern recognition steps. (e.g. Does the step response show first or second order dynamics ?) These are less easily automated. The library implemented by the author relies on rich, well-defined graphical output, to allow the modeller to accomplish the pattern identification steps.

5. MINIMUM VARIANCE CONTROL

The previous chapters have assembled the background necessary for modelling stochastic plants, via one specific method. This is perhaps useful in itself, but if we can predict plant behavior, then we should be able to obtain good control.

Consider once more the model:

$$y(k) = (\omega(z^{-1})/\delta(z^{-1}))\ z^{-(f+1)}\ u(k) + (\theta(z^{-1})/\phi(z^{-1}))a(k) \qquad (5.1)$$

where:

$y(k)$ = deviation from target
$u(k)$ = deviation from value which holds $y(k)$ at zero
f = pure process delay

Our problem is to derive a feedback controller:

$$u(k) = f(y(k)) \qquad (5.2)$$

which minimizes the variance in $y(k)$. For example, consider the case:

$$y(k) = \omega(0)u(k-1)+n(k) \qquad n(k)=(1-\theta z^{-1})/(1-\phi)\ a(k) \qquad (5.3)$$

For the noise to have no effect at the output, $y(k) = 0$. Then Equation (5.3) becomes:

$$u(k) = (-1/\omega(0))n(k+1) \qquad (5.4)$$

To make the control adjustment, we must somehow predict $n(k+1)$. From Equation (5.3):

$$n(k) = (1-\theta z^{-1})/(1-\phi z^{-1})a(k) \qquad (5.5)$$

which can be rewritten:

$$n(k+1) = \phi n(k) + a(k+1) - \theta a(k) \qquad (5.6)$$

Taking expectations at instant k we are left with:

$$\hat{n}(k+1) = \phi n(k) - \theta a(k) \qquad (5.7)$$

where we have used the fact that, at instant k, $E\{a(k+1)\} = 0$. Substituting for $n(k+1)$ in Equation (5.4):

$$u(k) = (-1/\omega(0))(\phi n(k)-\theta a(k)) \qquad (5.8)$$

Now, the best that this controller can do is:

$$y(k+1) = a(k+1) \qquad (5.9)$$

since the error in predicting $n(k+1)$ will show up in the output. That is, the minimum variance we can accomplish in this case is $\sigma^2(y) = \sigma^2(a)$. Substituting Equation (5.9) into (5.8), and using the noise model to substitute for $n(k)$ in terms of $a(k)$:

$$u(k) = (-1/\omega(0))(\phi-\theta)/(1-\phi z^{-1})\ y(k) \qquad (5.10)$$

which gives the control output in terms of the current plant output. Here, we have used the transfer function plus noise model to design a controller which will reject noise. In this derivation, we have implicitly assumed the desired process output (setpoint) to be zero. That is, we desire zero deviation from the steady-state value at which the model was developed. (Recall that both $y(k)$ and $u(k)$ represent deviations from steady-state.) Let us consider the case of a non-zero setpoint, say $y(k) = ysp(k)$. Now, if noise has no effect, $y(k) = ysp(k)$. Substituting this into Equation (5.3) and rearranging:

$$u(k) = (ysp_{k+1}/\omega(0)) - (n(k+1)/\omega(0)) \qquad (5.11)$$

The second term on the right will lead to the same result as before, so that the regulatory plus servo control law is:

$$u(k) = (ysp_{k+1}/\omega(0)) - (1/\omega(0))(\phi-\theta)\ /(1-\phi z^{-1})y(k) \qquad (5.12)$$

5.1 Analytical Derivation

When we derived the minimum variance controller for the first example, we took the following steps:

1. Set $y(k) = 0$, to obtain the control law from the transfer function plus noise model.
2. From the noise model, obtain the estimates $n(k+i)$ required in the control law.
3. Substitute these estimates to obtain the control law in terms of $a(k)$, $u(k)=g(a(k))$.
4. Obtain the relationship between $y(k)$ and $a(k)$ determined by the prediction errors.
5. Use this relationship to obtain the control law in terms of measurements $y(k)$, instead of the noise model inputs, $a(k)$.

This procedure may be entirely acceptable. However, we require a constructive proof to show that the controller will give minimum variance.

To begin, we require an expression for the variance of the plant output. We will then use analytic methods to derive the minimum variance control law.

Note that above, we were able to express $y(k)$ in terms of $a(k)$ alone. This should lead us to expect that the variance of $y(k)$ should be expressible in terms of the variance of $a(k)$.

Recall the original model:

$$y(k+f+1) = (\omega(z^{-1})/\delta(z^{-1}))u(k) + (\theta(z^{-1})/\phi(z^{-1}))a(k+f+1) \tag{5.13}$$

By definition, the transfer function is just an economical parameterization of the impulse response, $v(z^{-1})$, where:

$$v(z^{-1}) = \Sigma v(i)z^{-i} = (\omega(z^{-1})/\delta(z^{-1})) \qquad (5.14)$$

$$i = 0, \ldots, \infty$$

Substituting Equation (5.14) into (5.13):

$$y(k+f+1) = v(z^{-1})u(k) + (\theta(z^{-1})/\phi(z^{-1}))a(k+f+1) \qquad (5.15)$$

Recalling the third step in our heuristic procedure above, we should be able to express the control action in terms of the noise model inputs:

$$u(k) = \Sigma L(i)a(k-i) = L(z^{-1})a(k) \qquad (5.16)$$

$$i = 0, \ldots, \infty$$

Substituting Equation (5.16) into (5.15), we obtain $y(k)$ entirely in terms of $a(k)$:

$$y(k+f+1) = v(z^{-1})L(z^{-1})a(k) + (\theta(z^{-1})/\phi(z^{-1}))a(k+f+1) \qquad (5.17)$$

We saw earlier that it is possible to compensate for noise inputs occurring up to and including instant k. Certainly, all the terms in the first expression on the right side of Equation (5.17) fall into this category. We will have to cast the second term in a similar form to examine it more closely. Define the impulse response of the noise model:

$$\psi(z^{-1}) = \Sigma\psi(i)z^{-1} = \theta(z^{-1})/\phi(z^{-1}) \qquad (5.18)$$

$$i = 0, \ldots, \infty$$

Now separate this into two parts:

$$\psi(z^{-1}) = \psi_1(z^{-1}) + z^{-(f+1)}\psi_2(z^{-1}) \qquad (5.19)$$

so that $\psi_1(z^{-1})$ is of degree f, and $z^{-(f+1)}\psi_2(z^{-1})$ is the remaining high order part of $\psi(z^{-1})$. Then:

$$\psi(z^{-1})a(k+f+1) = \psi_1(z^{-1})a(k+f+1) + \psi_2(z^{-1})a(k) \qquad (5.20)$$

So $\psi_1(z^{-1})$ operates on disturbances which have not yet arisen at instant k. Now, substituting Equation (5.19) into (5.17):

$$y(k+f+1) = \{v(z^{-1})L(z^{-1}) + \psi_2(z^{-1})\}a(k) + \psi_1(z^{-1})a(k+f+1) \qquad (5.21)$$

Squaring:

$$\begin{aligned} y^2(k+f+1) = \{&[v(z^{-1})L(z^{-1})+\psi_2(z^{-1})]^2a^2(k) \\ &+ \psi_1(z^{-1})^2a^2(k+f+1) \\ &+[2v(z^{-1})L(z^{-1})\psi_1(z^{-1}) \\ &+ 2\psi_1(z^{-1})\psi_2(z^{-1})]a(k)a(k+f+1)\} \end{aligned} \qquad (5.22)$$

and taking expected values, we obtain:

$$\sigma^2(y) = \{\Sigma(v(i)L(i)+\psi_2(i))^2 + \Sigma\psi_1(i)^2\}\sigma^2(a) \qquad (5.23)$$

As required, we now have an expression for the variance of y(k). As mentioned above, it was possible to obtain this entirely in terms of a(k). And, as promised, we will now proceed to minimize this variance analytically.

First, we require one simple result. We defined the noise model impulse response as $\psi(z^{-1})$. That is:

$$\theta(z^{-1})/\phi(z^{-1}) = \psi(z^{-1}) \ , \ \psi(z^{-1}) = 1 + \psi_1 z^{-1} + \ldots \qquad (5.24)$$

Substituting from Equation (5.19):

$$\theta(z^{-1})/\phi(z^{-1}) = \psi_1(z^{-1}) + z^{-(f+1)}\ \psi_2(z^{-1}) \qquad (5.25)$$

At some point, we will have to determine $\psi_1(z^{-1})$ and $\psi_2(z^{-1})$. This can be looked at as a problem in polynomial division, where $\psi_2(z^{-1})$ gives the remainder terms. That is, we can define:

$$\psi_2(z^{-1}) = T(z^{-1})/\phi(z^{-1}) \ , \ T(z^{-1}) = T(0) + T(1)z^{-1} + \ldots \qquad (5.26)$$

We will need this result later. Let us pick up where we left off, in the minimization. The second sum in Equation (5.23) is independent of our actions. Only the first sum contains terms related to the control law. (This should not be surprising - recall that the second sum is related to as-yet unrealized disturbances.) So it will be sufficient to minimize the first sum. The minimum for a squared real value is zero, so we require:

$$\Sigma(v(i)L(i) + \psi_2(i))^2 = 0 \qquad (5.27)$$
$$\text{i.e. } v(z^{-1})L(z^{-1}) + \psi_2(z^{-1}) = 0$$

This will be satisified using the control law:

$$L(z^{-1}) = -\psi_2(z^{-1})/v(z^{-1}) \qquad (5.28)$$

This is a reasonable result. At the plant output, we could negate the disturbances with $-\psi_2(z^{-1})$. We move this action to the plant input by multiplying by the inverse of the plant transfer function.

Substituting Equation (5.28) into (5.16):

$$u(k) = -\psi_2(z^{-1})/v(z^{-1})\ a(k) \qquad (5.29)$$

Substituting for $v(z^{-1})$ from Equation (5.14), and for $\psi_2(z^{-1})$ from Equation (5.26):

$$u(k) = -(\delta(z^{-1})T(z^{-1}))/(\omega(z^{-1})\phi(z^{-1}))\ a(k) \qquad (5.30)$$

Now we are at a stage similar to the fourth step in the heuristic procedure. We have u(k) as a function of a(k), and would like u(k) as a function of y(k). Using the impulse response $\psi(z^{-1})$ in the original model, we have:

$$y(k) = (\omega(z^{-1})/\delta(z^{-1}))u(k-f-1) + \psi(z^{-1})a(k) \qquad (5.31)$$

Substituting for $\psi(z^{-1})$ from Equation (5.19), for $\psi_2(z^{-1})$ from Equation (5.26), and for u(k) from the control law,

Equation (5.30):

$$y(k) = \psi_1(z^{-1})a(k) \qquad (5.32)$$

As expected, the deviations are caused by the as-yet unrealized disturbances. Rearranging Equation (5.32) for a(k), and substituting into the control law, Equation (5.30):

$$u(k) = -\ (\delta(z^{-1})T(z^{-1}))/(\omega(z^{-1})\phi(z^{-1})\psi_1(z^{-1}))\ y(k) \qquad (5.33)$$

This is the minimum variance control law, written in terms of plant input and output.

5.2 Nonminimum Phase Systems

If $\omega(z^{-1})$ has zeroes on or inside the unit circle, the control law in Equation (5.33) will require infinite variance for the input u(k). Even if $\omega(z^{-1})$ is invertible, experience has shown that unacceptably large input variance may be called for. One solution is to add a constraint to the minimization. That is, minimize the output variance, $\sigma^2(y)$, subject to an upper bound on the input variance, $\sigma^2(u)$. For the problem:

$$\text{Min } \sigma^2(y) \text{ s.t. } \sigma^2(u) \le c\sigma^2(a) \qquad (5.34)$$

the method of Lagrangian multipliers leads to a minimization of:

$$F(u,y,\lambda) = \sigma^2(y) + \lambda(\sigma^2(u) - c\sigma^2(a)) \qquad (5.35)$$

Since we cannot effect $\sigma^2(a)$, this function will be minimum if:

$$G(u,y,\lambda) = \sigma^2(y) + \lambda\sigma^2(u) \qquad (5.36)$$

is minimum. Given that:

$$u(k) = \Sigma L(i)a(k-i) = L(z^{-1})a(k) \qquad (5.16)$$
$$i = 0, \ldots, \infty$$

the input variance can be expressed as:

$$\sigma^2(u) = \Sigma L^2(j)\sigma^2(a) \ , \ j = 0, \ldots, \infty \qquad (5.37)$$

Substituting from Equations (5.23) and (5.37) into Equation (5.36):

$$\begin{aligned} G(u,y,\lambda) = \{&\Sigma(v(i)L(i)+\psi_2(i))^2 \\ &+ \Sigma\psi_1^2(j) + \lambda\Sigma L^2(j)\}\sigma^2(a) \qquad (5.38) \\ &i = 0, \ldots, \infty \ j=0, \ldots, f \end{aligned}$$

Again, the second sum is independent of the control law, so we need only to minimize:

$$G(u,y,\lambda) = \{\Sigma(\psi_2(i)+\Sigma L(k)v(i-k))^2 + \lambda\Sigma L^2(i)\}\sigma^2(a) \qquad (5.39)$$
$$i = 0, \ldots, \infty \ k=0, \ldots, i$$

where the first summation has simply been rearranged. Differentiating, and since the first j terms are independent of L_j.

$$\begin{aligned} &\partial\Sigma(\psi_2(i)+\Sigma L(k)v(i-k))^2/\partial L(j) = \\ &\qquad 2\Sigma v(l-j)(\psi_2(l)+\Sigma L(k)v(l-k)) \qquad (5.40) \\ &\qquad i=0, \ldots, \infty \ l=j, \ldots, \infty \ k=0, \ldots, i \end{aligned}$$

Substituting Equation (5.40) into (5.38), differentiating the second term, and equating to zero:

$$\Sigma v(i-j)W(i)+\lambda L(j) = 0 \ , j\geq 0, \ i=j, \ldots, \infty \qquad (5.41)$$

where:

$$W(i) = \psi_2(i) + \Sigma L(k)v(i-k) \ , \ k=0, \ldots, i \qquad (5.42)$$

To get from the set of Equations (5.41) to the final form for the controller requires three somewhat involved steps. First, we will rewrite Equations (5.41) in operator form. Then we will perform a spectral factorization for the sum of two polynomials. Lastly, we use partial fractions to rearrange the equation. The reader may wish to leave these

steps for a second reading, and go directly to Equation (5.53)

This first manipulation is a rather elegant approach, due to Wilson (1969a).

The equations for the L_j can be solved much more easily if we can pass back to an operator notation. Consider:

$$v(z)W(z^{-1}) + \lambda L(z^{-1}) = H(z) \qquad (5.43)$$

where:

$$H(z) = \Sigma H(i)z^{i} \qquad i = -\infty, \ldots, \infty$$
$$W(z^{-1}) = L(z^{-1})v(z^{-1}) + \psi_2(z^{-1})$$

Expanding the left side, and equating coefficients of equal powers of z, we find that $H_i = 0$, $i \leq 0$, is required to satisfy Equations (5.41) The coefficients of H_i, $i > 0$, are not constrained by Equation (5.41), and will be left free. That is, we can embed the series problem of Equation (5.41) within the operator problem of Equation (5.43). Restating, our original definition was:

$$H(z) = \Sigma H(i)z^{i} \qquad i = -\infty, \ldots, \infty \qquad (5.44)$$

but Equations (5.41) constrain this to:

$$H(z) = \Sigma H(i)z^{i} \qquad i = 1, \ldots, \infty \qquad (5.45)$$

which is a power series in z, with a zero leading coefficient. Substituting from Equation (5.44) into (5.43):

$$v(z)\{L(z^{-1})v(z^{-1}) + \psi_2(z^{-1})\} + \lambda L(z^{-1}) = H(z) \qquad (5.46)$$

Substituting for $v(z^{-1})$ and $\psi_2(z^{-1})$ from Equations (5.14) and (5.26):

$$\frac{L(z^{-1})\omega(z)\omega(z^{-1}) + \lambda\delta(z)\delta(z^{-1})}{\delta(z)\delta(z^{-1})} + \frac{\omega(z)T(z^{-1})}{\delta(z)\phi(z^{-1})} = H(z) \qquad (5.47)$$

We now have two terms on the left, in various polynomials of z and z^{-1}. What we are after is a solution for $L(z^{-1})$. What

we require, then, is some way to disentangle the polynomials in z^{-1} from those in z. Let's start with the first term on the left. The spectral factorization theorem will let us perform the factorization as:

$$\omega(z)\omega(z^{-1}) + \lambda\delta(z)\delta(z^{-1}) = \gamma(z)\gamma(z^{-1}) \qquad (5.48)$$

where $\gamma(z^{-1})$ has no zeroes inside or on the unit circle. Further detail can be found in Wilson (1969b). Substituting from Equation (5.48) into (5.47):

$$\frac{L(z^{-1})\gamma(z)\gamma(z^{-1})}{\delta(z)\delta(z^{-1})} + \frac{\omega(z)T(z^{-1})}{\delta(z)\phi(z^{-1})} = H(z) \qquad (5.49)$$

Since $\gamma(z)$ is invertible, we can multiply by $\delta(z)/\gamma(z)$:

$$\frac{L(z^{-1})\gamma(z^{-1})}{\delta(z^{-1})} + \frac{\omega(z)T(z^{-1})}{\delta(z)\phi(z^{-1})} = H'(z) \qquad (5.50)$$

where, similar to H(z),:

$$H'(z) = \Sigma H'_i z^i \qquad i = 1, \ldots, \infty$$

Now, the first term is all in z^{-1}. Separating the second term by partial fractions:

$$\frac{-\omega(z)T(z^{-1})}{\gamma(z)\phi(z^{-1})} = \frac{Q_1(z^{-1})}{\phi(z^{-1})} + \frac{Q_2(z)}{\gamma(z)} \qquad (5.51)$$

where $Q_2(z)$ must have a zero constant term for uniqueness. Substituting from Equation (5.51) into (5.50):

$$\frac{L(z^{-1})\gamma(z^{-1})}{\delta(z^{-1})} - \frac{Q_1(z^{-1})}{\phi(z^{-1})} = \frac{Q_2(z) + H'(z)}{\gamma(z)} \qquad (5.52)$$

When expanded, the right side is a power series in z, with no constant term. The left side is a power series in z^{-1}. Thus, the equation is separable, and:

$$L(z^{-1}) = \frac{\delta(z^{-1})Q_1(z^{-1})}{\gamma(z^{-1})\phi(z^{-1})} \qquad (5.53)$$

Substituting Equation (5.53) into (5.16):

$$u(k) = \frac{\delta(z^{-1})Q_1(z^{-1})a(k)}{\gamma(z^{-1})\phi(z^{-1})} \qquad (5.54)$$

The interpretation of this equation is much less clear than for Equation (5.29). Recall the associated Equation (5.30):

$$u(k) = -\ (\delta(z^{-1})T(z^{-1}))/(\omega(z^{-1})\phi(z^{-1}))\ a(k) \qquad (5.30)$$

Looking at Equation (5.51), we note that $Q_1(z^{-1})$ is closely related to $T(z^{-1})$. The major change from Equation (5.30) to (5.54) has been the replacement of $\omega(z^{-1})$ by $\gamma(z^{-1})$. This is reasonable, since we were having problems with zeroes of $\omega(z^{-1})$ inside or on the unit circle. We can guarantee that $\gamma(z^{-1})$ will have all roots outside the unit circle. Once again, we are in the position of having a control law in terms of $a(k)$. Solving Equation (5.54) for $a(k)$, substituting into Equation (5.1), and rearranging for $u(k)$:

$$u(k) = \frac{\delta(z^{-1})Q_1(z^{-1})}{\omega(z^{-1})Q_1(z^{-1})z^{-(f+1)} + \gamma(z^{-1})\theta(z^{-1})}\,y(k) \qquad (5.55)$$

which is the final form for this controller. In this derivation, we have dealt directly with two common problems. First, non-minimum phase behavior has been accounted for. And excessive manipulation of the control input can be taken care of by the same approach.

5.3 Example

If we use the subroutine library to derive the unconstrained controller for the system modelled in section 4.7, we obtain:

$$u(k) = 2.698\frac{(z^{-1} - 14.73)(z^{-1} - 1.06)y(k)}{(z^{-1} + 1.132)(z^{-1} - 1.05)} \qquad (5.56)$$

Cancelling the approximate pair near the circle:

$$u(k) = \frac{-39.74y(k) + 2.698y(k-1) - u(k-1)}{1.132} \qquad (5.57)$$

Applying this controller, we obtain the results shown in Figure 5.1. Note that the transfer function has also been used to derive a servo controller, while variance from the target is minimized by the joint use of noise and transfer function models.

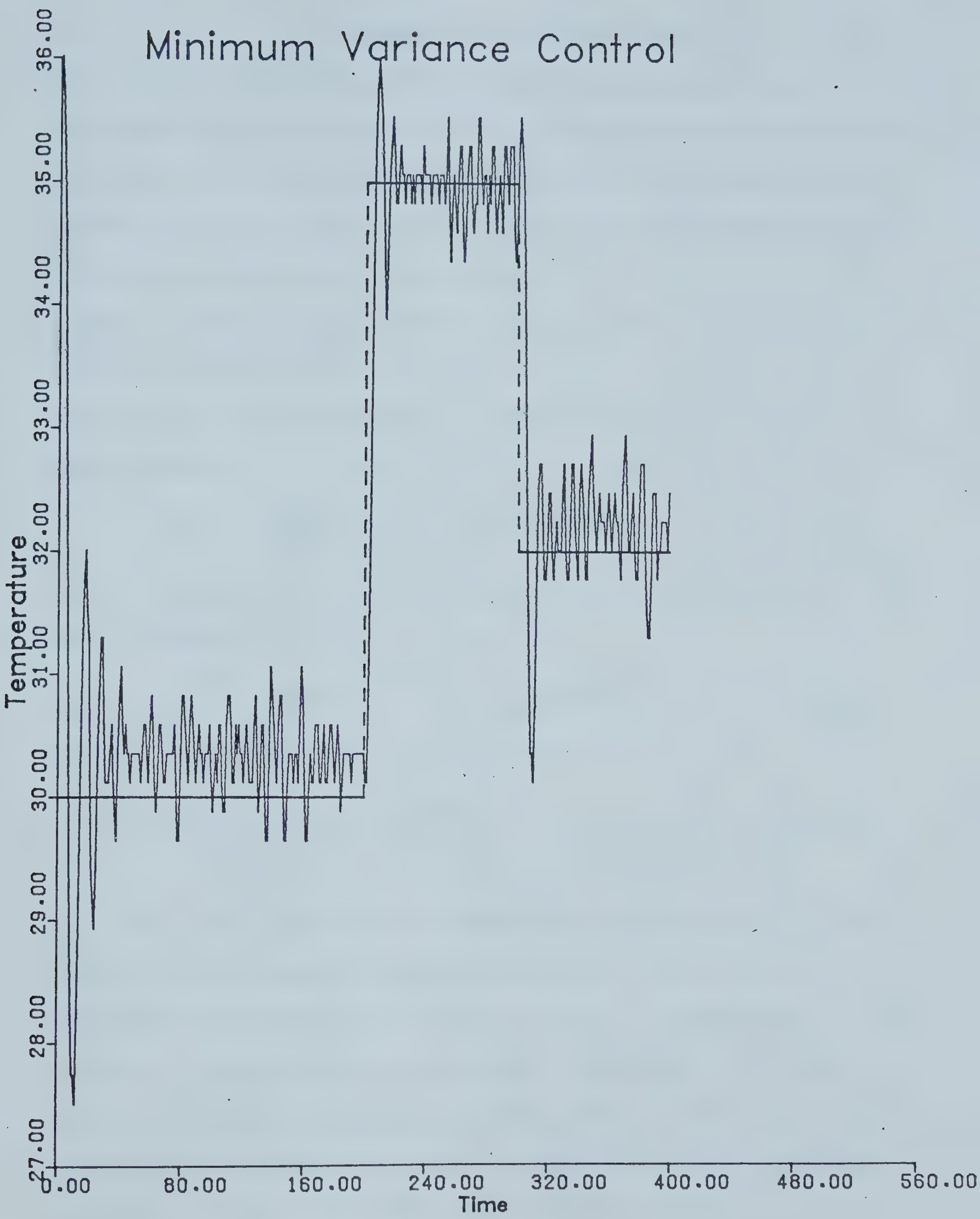

Figure 5.1 Controller Performance

6. SUMMARY AND OBSERVATIONS

This thesis was motivated, in the Introduction, by a consideration of the effects of improved regulatory control. This was followed by a consideration of the categories of models - in particular, state space and input-output models. Using the state space description :

$$\begin{aligned} x(k+1) &= \phi(k+1,k)x(k) + \Psi(k+1,k)u(k) + \Gamma(k+1,k)w(k) \\ y(k+1) &= H(k+1)x(k+1) \\ z(k+1) &= y(k+1) + v(k+1) \end{aligned} \qquad (2.1)$$

was stated to be equivalent to using the input-output description:

$$y(k) = \frac{B(z^{-1})}{A(z^{-1})} u(k) + \frac{C(z^{-1})}{A(z^{-1})} a(k) \qquad (2.3)$$

as a consequence of applying the Kalman filter theorem. This was generalized slightly to obtain:

$$y(k) = \frac{\omega(z^{-1})}{\delta(z^{-1})} z^{-b} u(k) + \frac{\theta(z^{-1})a(k)}{\phi(z^{-1})} \qquad (2.4)$$

where the polynomials are defined as:

$$\begin{array}{ll} \omega(z^{-1}) = \omega(0) - \Sigma\omega(i)z^{-i} & i = 1, \ldots, s \\ \delta(z^{-1}) = 1 - \Sigma\delta(i)z^{-i} & i = 1, \ldots, r \\ \theta(z^{-1}) = 1 - \Sigma\theta(i)z^{-i} & i = 1, \ldots, q \\ \phi(z^{-1}) = 1 - \Sigma\phi(i)z^{-i} & i = 1, \ldots, p \end{array} \qquad (2.5)$$

Then two approaches to developing such models - via frequency and impulse response methods - were defined. Basically, the difference between the two approaches is the domain of representation selected - frequency, or time. Next, the convolution integral was used to show that the correlation method is one way to perform impulse response analysis. It was also shown that the auto and cross-spectrum, used in frequency response analysis, are just Fourier transforms of their time-domain equivalents,

the auto and cross-correlation. Chapter 2 finished with an introduction of the path from nonparametric representations (e.g. impulse response), to parametric representations (e.g. transfer function). The iterative nature of the modelling process was emphasized, to ensure that the method to be presented would not be perceived as some sort of panacea. The observation was made that three major steps must be accomplished. First, we identify a candidate model structure. Then we estimate parameters for this structure. After evaluating the results, either the model is accepted, or we make a change and iterate through the process again.

In Chapter 3, the question of stability was considered, in conjunction with the noise model:

$$n(k) = \frac{\theta(z^{-1})}{\phi(z^{-1})} a(k) \qquad (3.2)$$

where

$$\begin{aligned} \theta(z^{-1}) &= 1 - \Sigma\theta_i z^{-i} \qquad i = 1, \ldots, q \\ \phi(z^{-1}) &= 1 - \Sigma\phi_i z^{-i} \qquad i = 1, \ldots, p \\ a(k) &= N(0,\sigma^2(a)) \end{aligned}$$

First, it was observed that the autoregressive (AR) and moving average (MA) operators are in some sense complementary. A finite order MA operator can be represented as an infinite order AR operator, and vice versa. Stationarity is defined as the convergence of an MA operator. Invertibility is defined as convergence of an AR operator. For finite order polynomial operators with bounded coefficients, convergence of the sum of coefficients is guaranteed. The issues of invertibility and stationarity arise only in the case of infinite order operators. So stationarity is important for infinite order MA operators,

that is, for finite order AR operators. And invertibility is important for infinite order AR operators, or finite order MA operators. In either case, the roots of the operator $\theta(z^{-1})$ or $\phi(z^{-1})$ must lie outside the unit circle for stability of the noise model.

Following this, the three basic tools for noise model identification were introduced. The autocovariance is related to the idea of variance. It is defined as:

$$\gamma(j) = E[n(k)n(k+j)] \tag{3.31}$$

and is estimated as:

$$c(j) = (1/N)\Sigma n(i)n(i+j) \quad i = 1, \ldots, N-j \tag{3.32}$$

To remove the dependance of this measure on the process variance, we normalize to obtain the autocorrelation:

$$r(j) = c(j)/c(0) \tag{3.34}$$

The autocorrelation will indicate the order of a pure MA process.

To determine the order of a pure AR process, the partial autocorrelation was defined. This measure is somewhat more of a made-to-order device, since the partial autocorrelation coefficients are actually best derived by fitting pure AR models of increasing degree to the data.

Neither the autocorrelation or partial autocorrelation will reveal the presence of periodicities in the data. This type of behavior can be investigated with the power spectrum of the data. The procedure here is to fit a Fourier series model:

$$n(k) = \alpha(0) + \Sigma(\alpha(i)c(i,k) + \beta(i)s(i,k) + e(k) \;, \; i=1, \ldots q \tag{3.52}$$

where:

$$c(i,k) = \cos(2\pi f(i)k)$$
$$s(i,k) = \sin(2\pi f(i)k) \quad f(i) = (i/N)$$

and then to represent the intensity at each frequency:

$$I(f(i)) = (N/2)(a^2(i) + b^2(i)) \quad i=1, \ldots, q \qquad (3.54)$$

graphically, versus frequency. If there are periodic components in the series, the power spectrum will show an increase of intensity in the vicinity of the frequencies of these components.

Following examples of the use of these tools for pure and mixed processes, it was then noted that to identify the noise model (i.e. to actually calculate the functions above), we must be able to partition the observations between the transfer function and noise model.

Continuing to work with nonparametric system representations in Chapter 4, the connection between cross-correlation and impulse response was examined in some detail. It was shown that the cross-correlation from input to output is the convolution of the autocorrelation of the input signal with the system impulse response. Given that we have an input-output series, deconvolution can be used to obtain an estimate of the impulse response. This will not necessarily be an efficient estimate, but it will allow identification of the noise model structure. A type of deconvolution called prewhitening was examined in this respect.

With an estimate for the noise series in hand, we can identify the noise model structure. We can also identify the

transfer function structure as a result of this same development. Once the output series can be partitioned into transfer function and noise model contributions, each part can be identified. The noise model is identified via the previously considered autocorrelation, partial autocorrelation and power spectrum. The transfer function is identified via the impulse or step response.

With an identified model in hand, we can proceed to parameter estimation. This is done via nonlinear least squares. The algorithm used is a version of Gauss' method, called the Levenburg - Marquardt correction:

$$x_{i+1} = x_i - C^{-1}_i [C^{-1}_i J_i^T J_i C^{-1}_i + \lambda I]^{-1} C^{-1}_i J_i^T Q_i \tag{4.46}$$

and we let:

$$\lambda_{i+1} = \lambda_i / \nu \tag{4.48}$$

where ν is a constant greater than 1. The Jacobian in the above equation can be estimated numerically, or calculated analytically. The library routine developed uses analytical calculations, since the model structure is fairly simple.

The model, once obtained, is only a means to an end. It can be used, for example, to understand the behavior of the plant within the range of the test data. It can also be used for better control. The noise model can be used to anticipate the effects of correlated disturbances. By using it to derive a regulator, minimum variance about a setpoint can be obtained. Special methods are required where the variance of the regulator's output is too high, or when the process is nonminimum phase. The transfer function model can

of course, also be used to advantage, for servo control. The simplest technique is to simply invert the transfer function, which is the method used in the last chapter. There are much more robust approaches.

What are the shortcomings of the method?

The major problem is the requirement for on-line, open-loop testing of the plant, to obtain an input-output series. This is objectionable in an industrial environment where risks to people, the surrounding community, equipment and profitability all must be considered. The requirement for open-loop testing arises from the assumption that the input and noise are not cross-correlated. In closed-loop, plant input is a function of control error, which is in turn correlated with the disturbances.

What can the method contribute?

Used as intended, the method is capable of delivering a transfer function plus noise model which can be used both for a basic understanding of the plant, and for improved control.

When compared to on-line methods, the most obvious difference is the emphasis on diagnostic checks. It is certainly possible to follow on-line the autocorrelation of the control error (analogous to residuals in the off-line analysis). The control errors should not be autocorrelated - if they are, there is some deficiency in the regulator. The autocorrelation of the control errors should be distributed as $\chi^2(\nu)$. And the power spectrum of the control errors

should be white.

Philosophically, the method has at least two things to contribute. First, it can be used as a stepping-off place to the topic of adaptive control. Secondly, it can be used as an introduction to stochastic processes. (e.g. Does the noise model represent the imperfect representation of the plant by the transfer function? Or does it represent something inherent in the system?) Both of these topics, to say nothing of the related area of time series analysis, can profitably be studied at length.

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APPENDIX A. TIME SERIES MODELLING

In Chapter 3, it was suggested that the model:

$$\nabla^{d} n(k) = (\theta(z^{-1})/\phi(z^{-1}))\ a(k) \qquad (A.1)$$

can generate a series of observations which appear to follow some pattern. However, this remark was made in the context of transfer function modelling. That is, we were considering:

$$y(k) = (\omega(z^{-1})/\delta(z^{-1}))z^{-}\ u(k) + n(k) \qquad (A.2)$$

where there is an implied causal relationship between u(k) and y(k). In contrast, models such as Equation (A.1) can be used to forecast a variable (e.g. a stock price) without specifying any causal relationship to another observable. This is referred to as time series modelling.

The subroutine package referred to previously provides the necessary tools for pure time series modelling.

The modelling procedure is similar to that for transfer function modelling. First, the autocorrelation, partial autocorrelation and power spectrum of the series must be considered, in order to find the model structure.

Given the model structure, the next step is to estimate the model parameters. This process can be simplified by the availability of reasonable initial guesses.

Consider the mixed ARMA(p,q) process:

$$n(k) = \phi(1)n(k-1)+\ldots+\phi(p)n(k-p) + a(k)-\theta(1)a(k-1)-\ldots$$
$$-\theta(q)a(k-q) \qquad (A.3)$$

Multiplying by n(k-i) and taking expectations:

$$\gamma(i) = \phi(1)\gamma(i-1)+\ldots+\phi(p)\gamma(i-p)$$

$$+ \gamma(n,a,i)-\theta(1)\gamma(n,a,i-1)-\ldots\theta(q)\gamma(n,a,i-q) \quad (A.4)$$

Given:

$$\gamma(n,a,i) = 0 \quad i>0$$
$$\gamma(n,a,i) \neq 0 \quad i\leq 0$$

Then:

$$\gamma(i) = \phi(1)\gamma(i+1)+\ldots+ \phi(p)\gamma(i-p) \quad k\geq q+1$$

In matrix form:

$$G\Phi = \Gamma$$

where:

$$\Phi = [\phi(1)\ldots\phi(p)]$$
$$\Gamma = [c(q+1)\ldots c(q+p)]$$
$$[g_{ij}] = c(|q+i-j|) \quad i,j = 1, \ldots, p$$

So that the initial estimates for the autoregessive parameters are readily available from these equations, known as the Yule-Walker equations.

Once the estimates are available, we can rewrite Equation (A.3) as:

$$-\phi(0)n(k)-\phi(1)n(k-1)-\ldots-\phi(p)n(k-p) =$$

$$a(k)-\theta(1)a(k-1)-\ldots-\theta(q)a(k-q) \quad \phi(0)=-1$$

Let:

$$w(k) = a(k)-\theta(1)a(k-1)-\ldots-\theta(q)a(k-q)$$

be the moving average part of the process, so that:

$$w(k) = -\phi(0)n(k)-\phi(1)n(k-1)-\ldots-\phi(p)\ n(k-p)$$

Multiplying by w(k-i) and taking expectations:

$$\hat{c}(w,w,i) = \Sigma\Sigma\phi(l)\phi(m)\ c(n,n,|i+l-m|) \quad \begin{array}{l} i=0,\ldots,q \\ l,m=0,\ldots,p \end{array} \quad (A.5)$$

We also have:

$$w(k) = a(k)-\theta(1)a(k-1)-\ldots-\theta(q)a(k-q) \quad a(k) = N(0,\sigma^2(a))$$

which can be rewritten as:

$$w(k) = \tau(0)e(k)\tau(1)e(k-1)+\ldots+\tau(q)e(k-q)$$
$$e(k) = N(0,1)$$

$$\theta(i) = -\tau(i)/\tau(0) \qquad i=1,\ldots,q$$
$$\sigma^2(a) = \tau(0)$$

Multiplying this by w(k-i) and taking expectations:

$$c(w,w,k) = \Sigma\tau(j)\tau(j+k) \qquad \begin{array}{l} i=0,\ldots,q \\ j=0,\ldots,q-i \end{array} \qquad (A.6)$$

Then the initial estimates of the moving average parameters are available by iterating on τ (e.g. Newton-Raphson), to solve:

$$\hat{c}(w,w,i) = c(w,w,i)$$
$$\Sigma\tau(j)\tau(j+i) - \hat{c}(w,w,i) = 0$$

For more details, see Wilson (1969b).

Given the model structure, plus a starting point, we can perform a regression to estimate the parameters. But, for the class of models we have chosen, the sum of squares is nonlinear with respect to some of the parameters.

Let [a(k)] denote E[a(k)], the expected value of the model residuals. For a pure autoregressive process:

$$[a(k)] = \phi(z^{-1})n(k)$$

so that

$$\partial[a(k)]/\partial\phi(i) = -[n(k-i)] + \phi(z^{-1})\partial[n(k)]/\partial\phi(i)$$

For $t > 0$, $[n(k)] = n(k)$, and $\partial[n(k)]/\partial\phi_i = 0$. So:

$$\partial[a(k)]/\partial\phi(i) = -n(k-i)$$

which is linear in ϕ.

For a pure moving average process:

$$[a(k)] = \theta^{-1}(z^{-1})n(k)$$
$$\partial[a(k)]/\partial\theta(i) = -\theta^{-2}(z^{-1})[n(k-j)] + \theta^{-1}(z^{-1})\partial[n(k)]/\partial\theta(j)$$

which is nonlinear in θ.

Our approach will be a variation of Gauss' method:

$$X_{i+1} = X_i - (J_i^T J_i)^{-1} J_i^T P_i$$

where:

X is the parameter vector

J is the Jacobian of the objective function

P is the vector of residuals

The Marquardt-Levenburg correction is to substitute:

$$(J_i^T J_i + \lambda_i I)^{-1} \qquad \lambda_{i+1} = \lambda_i/\nu$$

for $J^T J$ above. This ensures that the Hessian will remain positive definite during the approach to the extremum. This ensures invertibility. It also requires discretion in our choice of λ_0 and ν. Typically, λ_0 should be chosen to give an initial condition number of about 1, for $(J^T J+\lambda I)$. The constant ν should be chosen so that the condition number stays below about 100.

Box and Jenkins further stabilize the algorithm by using:

$$X_{i+1} = X_i - D(DJ^T JD + \lambda I)^{-1} DJ^T P$$

where D is the inverse of the purely diagonal matrix composed of the square root of the diagonal of J.

Of course, the objective function being minimized is the sum of squared residuals. However, we need more than just a choice for the parameter values to be able to calculate the residuals.

The general ARMA(p,q) model can be written:

$$a(k) = n(k) - \phi(1)n(k-1)-\ldots-\phi(p)n(k-p) + \theta(1)a(k-1)+\ldots+\theta(q)a(k-q)$$

To start this model, we need the p values of n(k), and q values of a(k) which occurred previous to the recorded

series.

One possibility is to set the unknown values equal to their expected values:

$$E[a(k)] = 0 \quad E[n(k)] = 0 \quad k<0$$

A second possibility which assumes less is to start the calculation from $k = p+1$, and set:

$$E[a(k)] = 0 \quad k \le p$$

The resulting loss of information is acceptable for large sample sizes. However, we do have the option of calculating the sum of squares without making any of these assumptions.

The general ARMA(p,q) model can be written in two equivalent forms:

$$\phi(z^{-1})n(k) = \theta(z^{-1})a(k) \tag{A.7}$$

$$\phi(z)n(k) = \theta(z)e(k) \tag{A.8}$$

We first use:

$$[e(k)] = \phi(z)n(k) + \theta(1)[e(k+1)] +\ldots+\theta(q)[e(k+q)]$$

to generate values for $e(k)$, where:

$$[e(k)] = 0 \quad t>N-p$$

Then:

$$[n(k)] = \phi(1)n(k+1)+\ldots+\phi(p)n(k+p) + \theta(z)e(k) \quad e(k)=0 \ , \ k\le 0$$

is used to generate $n(k)$ for $k=0, \ldots, -Q$. Because $\phi(z^{-1})$ is stationary, these estimates approach zero at some instant, $k = -Q$. Lastly,

$$[a(k)] = \phi(z^{-1})n(k)+\theta(1)a(k-1)+\ldots+\theta(q)a(k-q)$$

$$a(k)=0 \ , \ k\le -Q$$

is used to generate the residuals for $t = -Q,\ldots,N$. As well as the objective function, we must evaluate the Jacobian.

Given the simplicity of the models being used, it is relatively easy to use analytical rather than approximate derivatives. Recall:

$e(i) = n(i)-\phi n(i+1)-\ldots-\phi(p)n(i+p) +\theta(1)e(i+1)\ldots+\theta(q)e(i+q)$

So:

$$\frac{\partial e(i)}{\partial\theta(j)} = \frac{\partial n(i)}{\partial\theta(j)} - \frac{\phi(1)\partial n(i+1)}{\partial\theta(j)} - \ldots - \frac{\phi(p)\partial n(i+p)}{\partial\theta(j)}$$
$$+\frac{\theta(1)\partial e(i+1)}{\partial\theta(j)} + \ldots + \frac{\theta(q)\partial e(i+q)}{\partial\theta(j)} + \frac{e(i+j)}{\partial\theta(j)}$$

$$\frac{\partial e(i)}{\partial\phi(j)} = \frac{\partial n(i)}{\partial\phi(j)} - \frac{\phi(1)\partial n(i+1)}{\partial\phi(j)} - \ldots - \frac{\phi(p)\partial n(i+p)}{\partial\phi(j)}$$
$$+\frac{\theta(1)\partial e(i+1)}{\partial\phi(j)} + \ldots + \frac{\theta(q)\partial e(i+q)}{\partial\phi(j)} - \frac{n(i+j)}{\partial\phi(j)}$$

But given the N observations of n(i):

$$\partial n(i)/\partial\theta(j) = \partial n(i)/\partial\phi(j) = 0 \qquad i=1, \ldots, N$$

So that:

$$\frac{\partial e(i)}{\partial\theta(j)} = \frac{\theta(1)\partial e(i+1)}{\partial\theta(j)} + \ldots + \frac{\theta(q)\partial e(i+q)}{\partial\theta(j)} + e(i+j)$$

$$\frac{\partial e(i)}{\partial\phi(j)} = \frac{\theta(1)\partial e(i+1)}{\partial\phi(j)} + \ldots + \frac{\theta(q)\partial e(i+q)}{\partial\phi(j)} - n(i+j)$$

which can be used to backforecast the derivatives for i = N-p,...,1 by using the expectations:

$$e(i) = \partial e(i)/\partial\theta(j) = \partial e(i)/\partial\phi(j) = 0 \qquad i>N-p$$

Then we can backforecast the starting values:

$$\frac{\partial n(i)}{\partial\theta(j)} = \frac{\phi(1)\partial n(i+1)}{\partial\theta(j)} + \ldots + \frac{\phi(p)\partial n(i+p)}{\partial\theta(j)}$$
$$+ \frac{\partial e(i)}{\partial\theta(j)} - \frac{\theta(1)\partial e(i+1)}{\partial\theta(j)} - \ldots - \frac{\theta(q)\partial e(i+q)}{\partial\theta(j)} - \frac{e(i+j)}{\partial\theta(j)}$$

$$\frac{\partial n(i)}{\partial\phi(j)} = \frac{\phi(1)\partial n(i+1)}{\partial\phi(j)} + \ldots + \frac{\phi(p)\partial n(i+p)}{\partial\phi(j)}$$
$$+ \frac{\partial e(i)}{\partial\phi(j)} - \frac{\theta(1)\partial e(i+1)}{\partial\phi(j)} - \ldots - \frac{\theta(q)\partial e(i+q)}{\partial\phi(j)} + \frac{n(i+j)}{\partial\phi(j)}$$

for $i = 0,\ldots,-Q$, given:

$$\partial n(i)/\partial\theta(j) = \partial n(i)/\partial\phi(j) = 0 \qquad i = 1, \ldots, N$$

$$e(i) = \partial e(i)/\partial\phi(j) = \partial e(i)/\partial\theta(j) = 0 \qquad i \le 0$$

Finally, the required derivatives can be forecast:

$$\frac{\partial a(i)}{\partial\theta(j)} = \frac{\partial n(i)}{\partial\theta(j)} - \frac{\phi(1)\partial n(i-1)}{\partial\theta(j)} - \ldots - \frac{\phi(p)\partial n(i-p)}{\partial\theta(j)} + \frac{\theta(1)\partial a(i-1)}{\partial\theta(j)} + \ldots + \frac{\theta(q)\partial a(i-q)}{\partial\theta(j)} + \frac{a(i-j)}{\partial\theta(j)}$$

$$\frac{\partial a(i)}{\partial\phi(j)} = \frac{\partial n(i)}{\partial\phi(j)} - \frac{\phi(1)\partial n(i-1)}{\partial\phi(j)} - \ldots - \frac{\phi(p)\partial n(i-p)}{\partial\phi(j)} + \frac{\theta(1)\partial a(i-1)}{\partial\phi(j)} + \ldots + \frac{\theta(q)\partial a(i-q)}{\partial\phi(j)} - \frac{n(i-j)}{\partial\phi(j)}$$

given:

$$\partial n(i)/\partial\theta(j) = \partial n(i)/\partial\phi(j) = 0 \qquad i=1, \ldots, N$$

$$a(i) = \partial a(i)/\partial\theta(j) = \partial a(i)/\partial\phi(j) = 0 \qquad i<-Q$$

The use of these rather exacting calculations makes it possible to tackle small sample problems with confidence.

After obtaining a set of parameter estimates, several tests can be applied to determine their adequacy. First, the plot of residuals should be inspected, looking for any unusual features.

Second, the autocorrelation of the residuals should contain no significant terms.

We can also consider the first i autocorrelations as a group. If the fitted model is appropriate:

$$Q = N\Sigma r_j^2 \qquad j = 1, \ldots, i$$

should be distributed as $\chi^2(i-p-q)$.

Lastly, the power spectrum of the residuals should be white.

If more than one model can pass all the diagnostic tests, then the model with least parameters should be accepted.

Time series models can be useful for highly complex systems, which do not yield initially to a more descriptive analysis. In such situations, their predictive power can be very useful. Using this approach, a wide variety of phenomenae can be investigated. But the basic assumption of the method is that the observed behavior is the result of a random input to a linear filter. So any investigation of causal relationships will have to rely instead on something like transfer function modelling, with or without a stochastic element. This topic is covered in detail in the main body of this thesis.

APPENDIX B. TEST DATA

This file contains data from the stirred tank heater, with inputs made to the steam valve every 5 seconds, and tank temperature read at the same time. The DP for the water flow was also read. The data is recorded below as: temperature (DegC), steam valve position (%), DP (mm. Hg), in format 3E15.5 .

```
0.42533E+02    0.00000E+00    0.81216E+03
0.41837E+02    0.80000E+02    0.81510E+03
0.41606E+02    0.71000E+02    0.82981E+03
0.42764E+02    0.24000E+02    0.83570E+03
0.42996E+02    0.53000E+02    0.83570E+03
0.42069E+02    0.58000E+02    0.81216E+03
0.42069E+02    0.52000E+02    0.80980E+03
0.41606E+02    0.56000E+02    0.83570E+03
0.41606E+02    0.64000E+02    0.83276E+03
0.41837E+02    0.75000E+02    0.83570E+03
0.42764E+02    0.56000E+02    0.82393E+03
0.43227E+02    0.17000E+02    0.82981E+03
0.42533E+02    0.37000E+02    0.81804E+03
0.41837E+02    0.45000E+02    0.80686E+03
0.40909E+02    0.41000E+02    0.80686E+03
0.39979E+02    0.23000E+02    0.82687E+03
0.39047E+02    0.71000E+02    0.83570E+03
0.39047E+02    0.70000E+02    0.82981E+03
0.39979E+02    0.38000E+02    0.80098E+03
```

```
0.39746E+02    0.54000E+02    0.83570E+03
0.39513E+02    0.20000E+02    0.83805E+03
0.38814E+02    0.39000E+02    0.81804E+03
0.37647E+02    0.44000E+02    0.80392E+03
0.36945E+02    0.12000E+02    0.84394E+03
0.36009E+02    0.40000E+02    0.83805E+03
0.35070E+02    0.37000E+02    0.82687E+03
0.34365E+02    0.30000E+02    0.81216E+03
0.33659E+02    0.20000E+02    0.81216E+03
0.32481E+02    0.63000E+02    0.82393E+03
0.32481E+02    0.40000E+02    0.82687E+03
0.32717E+02    0.34000E+02    0.82393E+03
0.32717E+02    0.40000E+02    0.81216E+03
0.32009E+02    0.70000E+01    0.83570E+03
0.31300E+02    0.71000E+02    0.81804E+03
0.31300E+02    0.00000E+00    0.82393E+03
0.31536E+02    0.53000E+02    0.82393E+03
0.31064E+02    0.35000E+02    0.82981E+03
0.31300E+02    0.56000E+02    0.82687E+03
0.31536E+02    0.48000E+02    0.82981E+03
0.31773E+02    0.35000E+02    0.82687E+03
0.31773E+02    0.38000E+02    0.82687E+03
0.31536E+02    0.67000E+02    0.81216E+03
0.32009E+02    0.38000E+02    0.82393E+03
0.32481E+02    0.19000E+02    0.82981E+03
0.31536E+02    0.52000E+02    0.82687E+03
0.31300E+02    0.82000E+02    0.82687E+03
```

```
0.32953E+02    0.30000E+02    0.83570E+03
0.33895E+02    0.86000E+02    0.86395E+03
0.34365E+02    0.29000E+02    0.84688E+03
0.34835E+02    0.16000E+02    0.82687E+03
0.33895E+02    0.29000E+02    0.82393E+03
0.32953E+02    0.33000E+02    0.81510E+03
0.32245E+02    0.32000E+02    0.82393E+03
0.31300E+02    0.56000E+02    0.81216E+03
0.31536E+02    0.47000E+02    0.83570E+03
0.32009E+02    0.68000E+02    0.83570E+03
0.33188E+02    0.94000E+02    0.80392E+03
0.34835E+02    0.81000E+02    0.82393E+03
0.37413E+02    0.35000E+02    0.84982E+03
0.38348E+02    0.26000E+02    0.80686E+03
0.37179E+02    0.60000E+01    0.81510E+03
0.36009E+02    0.62000E+02    0.83805E+03
0.35540E+02    0.52000E+02    0.83570E+03
0.36009E+02    0.65000E+02    0.81216E+03
0.36711E+02    0.64000E+02    0.82099E+03
0.37413E+02    0.75000E+02    0.81804E+03
0.38814E+02    0.56000E+02    0.80686E+03
0.39513E+02    0.68000E+02    0.80980E+03
0.40212E+02    0.49000E+02    0.84100E+03
0.40444E+02    0.76000E+02    0.80686E+03
0.41141E+02    0.44000E+02    0.81216E+03
0.41373E+02    0.43000E+02    0.84688E+03
0.40909E+02    0.59000E+02    0.83276E+03
```

0.40909E+02	0.63000E+02	0.81216E+03
0.41141E+02	0.35000E+02	0.81216E+03
0.40677E+02	0.93000E+02	0.81216E+03
0.41606E+02	0.58000E+02	0.83805E+03
0.42069E+02	0.30000E+02	0.83805E+03
0.42069E+02	0.32000E+02	0.82099E+03
0.41141E+02	0.70000E+02	0.81510E+03
0.40909E+02	0.23000E+02	0.81804E+03
0.40677E+02	0.60000E+02	0.83570E+03
0.39979E+02	0.55000E+02	0.83570E+03
0.40212E+02	0.21000E+02	0.83805E+03
0.39513E+02	0.62000E+02	0.82393E+03
0.39047E+02	0.36000E+02	0.81510E+03
0.38814E+02	0.27000E+02	0.81804E+03
0.38114E+02	0.41000E+02	0.81510E+03
0.36945E+02	0.42000E+02	0.81216E+03
0.36477E+02	0.56000E+02	0.84100E+03
0.36243E+02	0.37000E+02	0.83805E+03
0.35774E+02	0.23000E+02	0.81804E+03
0.35070E+02	0.33000E+02	0.82393E+03
0.34130E+02	0.00000E+00	0.83276E+03
0.32953E+02	0.32000E+02	0.82099E+03
0.31536E+02	0.27000E+02	0.82393E+03
0.30827E+02	0.76000E+02	0.80392E+03
0.31536E+02	0.38000E+02	0.82687E+03
0.32009E+02	0.52000E+02	0.83805E+03
0.32245E+02	0.48000E+02	0.83570E+03

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0.32481E+02     0.60000E+02     0.83276E+03
0.32953E+02     0.52000E+02     0.82393E+03
0.33424E+02     0.24000E+02     0.82981E+03
0.33188E+02     0.67000E+02     0.81510E+03
0.33659E+02     0.42000E+02     0.82099E+03
0.33895E+02     0.56000E+02     0.81804E+03
0.34130E+02     0.63000E+02     0.81216E+03
0.34835E+02     0.54000E+02     0.81510E+03
0.35070E+02     0.62000E+02     0.81510E+03
0.35540E+02     0.84000E+02     0.82981E+03
0.37179E+02     0.23000E+02     0.83570E+03
0.37881E+02     0.25000E+02     0.78685E+03
0.36945E+02     0.80000E+02     0.84982E+03
0.37179E+02     0.91000E+02     0.82393E+03
0.39047E+02     0.52000E+02     0.83276E+03
0.40212E+02     0.73000E+02     0.82393E+03
0.40909E+02     0.58000E+02     0.82099E+03
0.41141E+02     0.79000E+02     0.80686E+03
0.42533E+02     0.57000E+02     0.81510E+03
0.43227E+02     0.79000E+02     0.81510E+03
0.43920E+02     0.81000E+02     0.82393E+03
0.45305E+02     0.51000E+02     0.82099E+03
0.45995E+02     0.58000E+02     0.82981E+03
0.45995E+02     0.16000E+02     0.83276E+03
0.45074E+02     0.40000E+02     0.83570E+03
0.44151E+02     0.13000E+02     0.83570E+03
0.42069E+02     0.52000E+02     0.82099E+03
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0.41373E+02    0.68000E+02    0.81804E+03
0.41606E+02    0.82000E+02    0.82687E+03
0.42996E+02    0.67000E+02    0.83570E+03
0.43689E+02    0.27000E+02    0.80980E+03
0.43689E+02    0.92000E+02    0.82393E+03
0.43920E+02    0.55000E+02    0.82099E+03
0.44382E+02    0.54000E+02    0.82687E+03
0.44151E+02    0.28000E+02    0.82099E+03
0.43227E+02    0.41000E+02    0.86395E+03
0.42301E+02    0.67000E+02    0.82099E+03
0.42533E+02    0.50000E+02    0.80980E+03
0.42301E+02    0.46000E+02    0.80980E+03
0.41606E+02    0.69000E+02    0.82393E+03
0.42069E+02    0.74000E+02    0.83805E+03
0.42764E+02    0.51000E+02    0.81510E+03
0.43227E+02    0.75000E+02    0.81804E+03
0.43689E+02    0.34000E+02    0.81804E+03
0.43227E+02    0.15000E+02    0.82393E+03
0.42301E+02    0.69000E+02    0.82687E+03
0.42069E+02    0.62000E+02    0.82099E+03
0.42533E+02    0.62000E+02    0.80980E+03
0.42764E+02    0.70000E+01    0.81510E+03
0.42069E+02    0.39000E+02    0.82981E+03
0.41141E+02    0.51000E+02    0.82981E+03
0.40212E+02    0.29000E+02    0.82099E+03
0.39513E+02    0.41000E+02    0.82687E+03
0.38581E+02    0.60000E+02    0.81804E+03
```

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0.38581E+02    0.43000E+02    0.82099E+03
0.38348E+02    0.55000E+02    0.83276E+03
0.37881E+02    0.55000E+02    0.83276E+03
0.37881E+02    0.45000E+02    0.80686E+03
0.37647E+02    0.74000E+02    0.82393E+03
0.38348E+02    0.31000E+02    0.82099E+03
0.38581E+02    0.57000E+02    0.81804E+03
0.37881E+02    0.42000E+02    0.82393E+03
0.37881E+02    0.42000E+02    0.80392E+03
0.37179E+02    0.50000E+02    0.86689E+03
0.36945E+02    0.40000E+02    0.82687E+03
0.36477E+02    0.34000E+02    0.82393E+03
0.35540E+02    0.37000E+02    0.82393E+03
0.35070E+02    0.68000E+02    0.81510E+03
0.35070E+02    0.56000E+02    0.82393E+03
0.36009E+02    0.50000E+02    0.83276E+03
0.36009E+02    0.45000E+02    0.81804E+03
0.35774E+02    0.97000E+02    0.82981E+03
0.36945E+02    0.36000E+02    0.82099E+03
0.37413E+02    0.65000E+02    0.82099E+03
0.37647E+02    0.50000E+02    0.81804E+03
0.37881E+02    0.64000E+02    0.81216E+03
0.38114E+02    0.48000E+02    0.80980E+03
0.38114E+02    0.41000E+02    0.84688E+03
0.37881E+02    0.84000E+02    0.80980E+03
0.38581E+02    0.63000E+02    0.82099E+03
0.39746E+02    0.23000E+02    0.82393E+03
```

```
0.39746E+02    0.49000E+02    0.82393E+03
0.38814E+02    0.50000E+02    0.82099E+03
0.38348E+02    0.58000E+02    0.82687E+03
0.38581E+02    0.14000E+02    0.82393E+03
0.38348E+02    0.76000E+02    0.81510E+03
0.38114E+02    0.79000E+02    0.81510E+03
0.39746E+02    0.55000E+02    0.81510E+03
0.40212E+02    0.74000E+02    0.82393E+03
0.41141E+02    0.24000E+02    0.81804E+03
0.41373E+02    0.67000E+02    0.82687E+03
0.40909E+02    0.44000E+02    0.86395E+03
0.40909E+02    0.63000E+02    0.82981E+03
0.41141E+02    0.11000E+02    0.82099E+03
0.40444E+02    0.44000E+02    0.82393E+03
0.39513E+02    0.40000E+02    0.83276E+03
0.38581E+02    0.77000E+02    0.82099E+03
0.38814E+02    0.42000E+02    0.82393E+03
0.39047E+02    0.53000E+02    0.82393E+03
0.38814E+02    0.31000E+02    0.81804E+03
```